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ABSTRACT BOOK

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SIMP-SGI-SOGEI 2019

Il tempo del pianeta Terra
e il tempo dell'uomo:
Le geoscienze fra passato e futuro



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ABSTRACT INDEX

Sessioni Plenarie	35
Cordier P. - Creeping minerals: new insights from numerical modelling and transmission electron microscopy.....	36
Fantoni R. - The Po Plain - Adriatic foreland from Mesozoic extension to Cenozoic compression.....	37
Iadanza A., Tribuzio R. & CNR Committee “ECORD-IODP and ICDP” - IODP-Italia and the Italian participation in ECORD-IODP and ICDP.....	38
Luguet A. - Mantle Geochronology: Insights from the Re-Os isotopic system.....	39
S1. Integrated mineralogy, petrology and computational modelling to decipher geochemical interactions and tectonic histories recorded by metamorphic rocks from the deep Earth	40
Agrosi G., Tempesta G., Mele D., Caggiani M.C., Mangone A., Della Ventura G.C., Cestelli-Guidi M., Allegretta I., Hutchison M.T., Nimis P. & Nestola F. - Multiphase inclusions associated with residual carbonate shed new light on the origin of super-deep diamonds from Juina (Brazil).....	41
Bonazzi M., Tumiati S., Thomas J., Angel R.J. & Alvaro M. - Elastic geobarometry for Quartz inclusions in garnet: comparison between hydrostatic and isotropic methods to evaluate the entrapment pressures..	42
Cámara F., Lotti P., Belmonte D., Pagliaro F., Merlini M. & Joseph B. - High pressure softening of grossite (CaAl ₄ O ₇).....	43
Campomenosi N., Scambelluri M., Angel R.J., Hermann J., Rubatto D., Mihailova B. & Alvaro M. - Applying Raman-elastic barometry to UHP metamorphic rocks: insights from the Dora Maira Massif (Western Alps).....	44
Capizzi L.S., Stagno V., Andreozzi G.B., Bosi F., Nazzari M. & Scarlato P. - Experimental investigation of the stability of iron-rich tourmaline as a function of pressure, temperature and oxygen fugacity with implications for the release of B-rich fluid during subduction.....	45
Ferrero S., Angel R.J., O’Brien P.J. & Wunder B. - Mineral growth and metastability phenomena in melt inclusions from metamorphic rocks	46
Geddo Z., Mazzucchelli M.L. & Alvaro M. - Combining micro-tomography and finite element analyses for elastic geobarometry on real geological samples	47
Jahn S. - First-principles molecular dynamics simulations of aqueous fluids at high temperatures and pressures	48
La Fortezza M., Campione M., Alvaro M., Scambelluri M. & Malaspina N. - Multiphase inclusions in harzburgites from the Bétic Cordillera (Cerro de Almirez, Spain): growth and orientation of magnetite in olivine	49
Locatelli M., Verlaquet A., Agard P., Pettke P. & Federico L. - Stepwise brittle deformation at 80 km-depth triggered by internal then external fluid circulation (Monviso eclogitic breccias, W. Alps).....	50
Lorenzon S., Nestola F., Thomassot E., Prosperi L., Lorenzetti A., Alvaro M., Salvadego F. & Nimis P. - Super-deep diamond from Central African Republic.....	51
Morana M., Murri M., Girani A., Angel R. J. & Alvaro M. - Characterizing deviatoric stress in mineral inclusions.....	52
Musiyachenko K., Murri M., Prencipe M. & Alvaro M. - Rutile in diamond: the role of elastic anisotropy	53
Nestola F., Zaffiro G., Mazzucchelli M.L., Nimis P., Andreozzi G.B., Periotto B., Princivalle F., Lenaz D., Secco L., Pasqualetto L., Logvinova A.M., Sobolev N.V., Lorenzetti A. & Harris J.W. - Diamond-magnesiocromite host-inclusion system recording old deep lithosphere conditions at Udachnaya (Siberia).....	54
Pasqualetto L., Nestola F., Nimis P., Jacob D.E., Oliveira B., Perritt S., Chinn I., Milani S. & Harris J.W. - Crystallographic relationships between diamond and its clinopyroxene inclusions.....	55
Rebay G., Godard G. & Kiénast J.R. - Eclogite-facies coronitic metagabbro and metatroctolite from the Zermatt-Saas ophiolites, Valtournanche, Italy.....	56

Zhong X., Andersen N., Dabrowski M. & Jamtveit B. - Zircon and quartz inclusions in garnet used for complimentary Raman-thermobarometry: application to the Holsnøy eclogite, Bergen Arcs, Western Norway	57
S2. Mineralogical Crystallography and New Minerals	58
Agrosi G., Lacalamita M., Mesto E., Schingaro E. & Tempesta G. - New insights into the crystal chemistry of tourmaline from Busachi (central Sardinia), Italy.....	59
Bersani D., Fornasini L., Zanoni A., Andò S., Gentile P., Salvioli-Mariani E. & Lottici P.P. - Micro-Raman chemical characterization of amphiboles	60
Biagioni C., Bosi F., Cook N.J., George L.L., Makovicky E., Moëlo Y., Pasero M., Sejkora J., Stanley C.J. & Welch M.D. - New nomenclature and classification of tetrahedrite-group minerals	61
Biagioni C., Mauro D., Bindi L., Hålenius U. & Pasero M. - Giacovazzoite and scordariite, two new minerals related to metavoltine.....	62
Bindi L. - Collisions in outer space produced a vacancy-rich, partially inverted tetragonal ringwoodite in several shocked meteorites	63
Bonaccorsi E., Merlino S. & Pasero M. - Superstructure of moraesite: a synchrotron study	64
Bonazzi P. & Bindi L. - Dienerite, Ni ₃ As: a mineralogical species to revalidate	65
Bussolesi M., Zaccarini F., Grieco G. & Tzamos E. - Rare and new mineralogical phases in the Ni-Cu-Sb-As system from the Gomati ophiolite, Northern Greece	66
Carbone C., Audra P., De Waele J., Bentaleb I., Chro?áková A., Krišt?fek V., D'Angeli I.M., Madonia G., Vattano M., Scopelliti G., Cailhol D., Vanara N., Temovski M., Bigot J.-Y., Nobécourt J.-C., Galli E., Rull F. & Sanz-Arranz A. - Phosphate minerals forming in karst environment: a state of art	67
Consani S., Giuli G., Martinelli A., Cardinale A.M., Trapananti A. & Carbone C. - Possible Rare Earth Element-induced structural modification in Layer Double Hydroxides: the case of synthetic woodwardite [Cu _{1-x} Al _x (SO ₄) _{x/2} (OH) ₂ ?nH ₂ O]	68
Della Ventura G., El Moutouakkil N., Boukili B., Lucci F., Conte A. & Talavera C. - Tracking the Ti substitution in biotite by FTIR imaging	69
Della Ventura G., Hawthorne F.C., Waesermann N. & Mihailova B. - The quantitative analysis of the octahedral composition of amphiboles by Raman spectroscopy.....	70
Fantini R., Quartieri S., Arletti R., di Renzo F., Fabbiani M., Morandi S., Martra G. & Vezzalini G. - Dehydration and Thermal stability of High-Silica Mordenite: <i>In-Situ</i> Synchrotron X-Ray Powder Diffraction Study	71
Griffin W.L., Gain S.E.M., Camara F., Bindi L., Toledo V. & O'Reilly S.Y. - Exotic mineralogy in an ultra-reduced magmatic system beneath Mt Carmel, Israel.....	72
Lotti P., Comboni D. & Gatta G.D. - Unusual symmetry of an intermediate scapolite.....	73
Mauro D., Biagioni C., Pasero M. & Zaccarini F. - Coquimbite: a mineral to be redefined?	74
Mesto E., Laurita S., Lacalamita M., Schingaro E., Rizzo G., Sinisi R. & Mongelli G. - Crystal-chemistry and thermal behavior of Fe-carpholite: a case of study from the Pollino Massif (southern Italy).....	75
Mugnaioli E., Gemmi M. & Németh P. - Disorder and modulation in first aragonite precipitates from Obstanser Eishöhle (Austria).....	76
Nazzareni S., Nestola F., Bindi L., Scricciolo E., Pacheco J., Zanon V., Zanatta M. & Giuli G. - Peculiar mineralogy of the Água de Pau syenites (São Miguel, Azores islands, Portugal)	77
Precisvalle N., Martucci A., Ferretti V., Bonadiman C., Bianchini G. & Natali C. - A reexamination of the crystal structure of lorándite	78
Scricciolo E., Nazzareni S., Giura P., Calandrini E. & Giuli G. - IR and Single-crystal XRD characterisation of natural pyrochlores	79
Zucchini A., McCammon C., Comodi P. & Frondini F. - Ex situ study of cation disorder in Fe-rich dolomites	80

S3. Georesources, geomaterials and their synthetic counterparts: occurrence, properties, utilizations/industrial applications	81
Aquino A., Lezzerini M., Pecchioni E., Giamello M., Cantisani E. & Fratini F. - Production of hydraulic binders using Lime from Mt. Morello formation in Florence area (Tuscany, Italy)	82
Ardit M. & Dondi M. - Micronization of ceramic pigments: the mineralogist's viewpoint on comminution rate and amorphisation.....	83
Beltrami G. - Thermal stability of hybrid organic-inorganic metasilicates	84
Boschi C., Baneschi I., Bonini M., Brogi A., Dini A., Gola G., Lelli M., Liotta D., Norelli F., Manzella A., Montanari D., Montegrossi G., Orlando A., Raco B., Rielli A., Ruggieri G., Santilano A. & Trumpy E. - H2020 GECO - Geothermal Emission Control- Project.....	85
Carta R. & Fumanti F. - The Mineral resources database of Italy (GeMMA).....	86
Castagnotto E., Locardi F., Cabella R. & Ferretti M. - Purple hematite: synthesis of the pigment <i>Caput Mortuum</i> through thermal treatment of natural samples	87
Caviglia C., Confalonieri G., Destefanis E., Mandrone G., Pastero L., Boero R. & Pavese A. - Evaluations of the reuse of municipal solid waste incinerator bottom ashes as aggregated materials in civil applications.....	88
Chirico R., Mondillo N. & Boni M. - Preliminary characterization of the Nonsulfide Zn(Pb) ores from the Florida Canyon Project (Northern Peru)	89
Coccatto A., Strocchio A., Finocchiaro C., Fugazzotto M., Occhipinti R., Bersani D., Fornasini L., Mazzoleni P. & Barone G. - Raman spectroscopy of aluminosilicates. What about geopolymers?	90
Columbu S., Comboni D., Gatta G.D. & Sitzia F. - Chemical reactivity of pozzolans from Sardinia for the industrial production of hydraulic limes.....	91
Comboni D., Lotti P., Gatta G.D., Merlini M. & Hanfland M. - Anisotropic compressional behavior of ettringite.....	92
Comodi P., Cavalaglio G., Nicolini A., Cambi C., Vivani R., Zucchini A., Susta U., Frondini F. & Cotana F. - Biomass vs coal ashes: a multi-methodic analysis to assess their hazardousness or reusability	93
Confalonieri G., Arletti R., Di Renzo F., Fabbiani M., Fois E., Haines J., Martra G., Quartieri S., Santoro M., Tabacchi G. & Vezzolini G. - Hydrocarbon Polymerization in Pure Silica Mordenite: The Effects of Structure, Pressure, Temperature and Time.....	94
Conte S., Zanelli C., Melchiades F.G., Hernández-Sánchez M.Y., Boschi A.O. & Dondi M. - Brazilian phyllite as feldspar substitute in ceramic bodies	95
Dondi M., Guarini G., Conte S., Molinari C., Soldati R. & Zanelli C. - A global view at sourcing and composition of fluxes for ceramics.....	96
Ercoli R., Renzulli A., Orlando A., Tassi F., Pagnetti A., Vaselli O., Borrini D., Paris E., Tarantino S.C. & Di Gregorio A. - Enhancing the sustainability of the aluminium production: experimental tests addressed to the inertization of industrial by-products through hydrogen storage for furnace fuel and to the synthesis of foamed geopolymers.....	97
Finocchiaro C., Barone G., Mazzoleni P., Leonelli C. & Rossignol S. - FT-IR study of early stages of geopolymer gel formation of AAMs based on pyroclastic deposits (Mt. Etna, Sicily, Italy) using two different alkaline solutions	98
Fugazzotto M., Coccatto A., Finocchiaro C., Occhipinti R., Strocchio A., Mazzoleni P. & Barone G. - Red brick waste as geopolymeric precursor for a sustainable restoration of ancient masonry	99
Funari V., Mantovani L., Vigliotti L., Dinelli E. & Tribaudino M. - Municipal solid waste incineration (MSWI) ashes: potential impacts and metal resources assessed by environmental magnetic methods..	100
Gaggero L., Ferretti M. & Locardi F. - Assessment of post treatment acceptance for Asbestos-Containing Waste by differential thermal analysis and thermo-gravimetry (DTA-TG).....	101
Galderisi A., Iezzi G., Bianchini G., de Brito J., Paris E., Piattelli V., Casarin A., Cinosi J., Macrini D., Schettino D., Santone S., Rossi M. & Buccieri F. - Petrography of Construction and Demolition Wastes from Abruzzo Region (Italy)	102

Giorno M., Barale L., Bertok C., D’Atri A., Martire L., Piana F. & Rossetti P. - Gorno mining district (Southern Alps): new preliminary data about ore mineral precipitation and multiphase diagenetic evolution	103
Lotti P., Comboni D., Gatta G.D., Pagliaro F., Catizzone E., Migliori M., Giordano G., Milani S., Merlini M., Collings I.E. & Hanfland M. - Methanol intrusion in MFI- Zeolites at High Pressure	104
Mancinelli M., Pompilio A., de Castro E.I., Pasti L., Rosatelli G., Di Bonaventura G., Pedrotti J.J. & Martucci A. - Development of a nanocomposite membrane based on reduced graphene (r-GO) and zeolite 13X for the removal of metal ions with bactericidal actions	105
Mantovani L., Funari V., Tribaudino M., Mazzari C. & Sabatino S. - Bottom ash from Parma WtE plant: mineralogical and chemical characterization	106
Martucci A., Bonadiman C., Zappaterra O., Renna M., Castelli S. & Rodeghero E. - Traceability of Ruby: challenges and opportunities by a combined LA-ICP-MS, UV-VIS and XR diffraction.....	107
Moroni M., Naitza S., Rossetti P., Ruggieri G., Magnani L., Aquino A., Tartarotti P., Ferrari E., Oggiano G. & Secchi F. - Conditions for hydrothermal cobalt and nickel mineralization – suggestions from some little known, historical ore deposits in Italy	108
Moroni M., Sessa G., Tumiati S., Ferrari E. & Langone A. - Hydromagmatic PGE telluride-rich Ni-Fe-Cu sulfide mineralization related to melt-rock reaction processes in presence of carbonated hydrous fluids: examples from sulfide-rich ultramafic intrusions of the Ivrea-Verbano Zone.....	109
Naitza S., De Giudici G.B., Funedda A., Loi A., Meloni M.A., Moroni M., Oggiano G. & Secchi F. - Metallogenesis in Sardinia - the Critical Raw Materials (CRM) perspective	110
Novembre D., Gimeno D., Graziano S.F. & Cappelletti P. - Zeolitization processes at the pyroclastic deposit “Tufo rosso a scorie nere” (Auctorum), Vico Volcano, Italy.....	111
Novembre D., Gimeno D. & Del Vecchio A. - Synthesis and characterization of Li-ABW zeolite using a kaolinitic rock.....	112
Oberto M. & Rossetti P. - The gold mineralization of Rio Cannero (Serie dei Laghi, north-western Italian Alps): first geologic and metallogenic data	113
Occhipinti R., Coccato A., Finocchiaro C., Fugazzotto M., Strocio A., Mazzoleni P. & Barone G. - Natural-fibres-reinforced geopolymers for application in Cultural Heritage	114
Paris E., Grandinetti V., Manzi S., Stabile P. & Bignozzi M.C. - Geopolymer-based Terrazzo tiles with a high-waste content: stepping forward from the laboratory phase to the industrial scale	115
Peroni V., Botter R., Cabella R., Risso L. & Carbone C. - Mineralogical and microstructural characterization of stoneware for wine use.....	116
Polisi M., Fabbiani M., Arletti R., Vezzalini G., Martra G., Di Renzo F. & Quartieri S. - Zeolite as an abiotic environment for amino acid condensation: spatial confinement and high pressure effects	117
Precisvalle N., Martucci A., Bonadiman C., Langone A. & Nobre A. - Topaz characterization: mineralogy and geochemistry at the service of the jewelry market	118
Putzolu F., Abad I., Balassone G., Boni M., Cappelletti P., Graziano S.F., Maczurad M., Mondillo N., Najorka J. & Santoro L. - Genesis of phyllosilicates in the Wingellina Ni-Co laterite deposit (Western Australia).....	119
Rossi G., Gamberi F., Marani M., Mattioli M., Di Gregorio A. & Renzulli A. - The hydrogenetic ferromanganese crusts and hydrothermal massive sulphide deposits in the Tyrrhenian Seafloor: a geological reassessment of the supply of Raw Materials.....	120
Santoro L., Herrington R. & Putzolu F. - Natural Iron oxy-hydroxides from supergene ore deposits: mineralogical, morphological and geochemical characterization	121
Sinisi R., Mongelli G., Perri F. & Khosravi M. - Aluminum Phosphate–Sulfate (APS) minerals occurrence and REEs control in the Darzi-Vali bauxite deposit, Iran.....	122
Stabile P., Abudurehman A., Bello M., Carroll M.R. & Paris E. - Characterization and vitrification of combined waste materials and potential use for reutilization in eco-sustainable building	123
Toffolo L., Nimis P., Tret’yakov G.A., Melekestseva I.Yu. & Beltenev V.E. - What controls metal endowment of massive sulfide deposits on mid-ocean ridges?	124

Ulian G., Moro D. & Valdrè G. - Density Functional investigation of the thermomechanical, electronic and thermodynamic properties of ZnS cubic polymorphs	125
Ulian G., Moro D. & Valdrè G. - Thermal and mechanical properties of phyllosilicates: some case studies from <i>ab initio</i> quantum mechanical investigations.....	126
Zanelli C., Conte S., Molinari C., Soldati R., Guarini G. & Dondi M. - Geomaterials on the edge of the circular economy: the case study of the ceramic tile industry.....	127
S4. Minerals, environment and medical uses	128
Beltrami G., Martucci A., Pasti L. & Chenet T. - Probing the sorption capacity of Y Zeolite towards pharmaceutical compounds: a neutron powder diffraction study.....	129
Belviso C., Belviso S., Ragone P. & Cavalcante F. - Red mud neutralization by layered double hydroxides (LDHs) formation: differences in the synthesis process used	130
Botta S., Avataneo C., Barale L., Compagnoni R., Cossio R., Marcelli I., Piana F., Tallone S. & Turci F. - Petrofacies for the prediction of NOA content in rocks: application to the “Gronda di Genova” tunneling project.....	131
Capella S., Visonà S., Osculati A. & Belluso E. - Occupational and anthropogenic environmental exposure during asbestos-cement production by FIBRONIT in Broni (Pavia): assessment of asbestos lung burden by SEM-EDS	132
Chillieri E., Byrne P., Onnis P., Lattanzi P., Costagliola P., Rimondi V. - Trace metal contents and mobility in mine wastes of the Central Wales mine district: environmental implications.....	133
Croce A., Rinaudo C., Grosso F., Erra S. & Amisano M.F. - Identification of asbestos fibers in tissues of patients affected by important diseases in extra respiratory systems	134
D’Aleo R., Cangemi M., Speziale S., Garabeiti E., Madonia P. & Favara R. - Ash leachates from Yasur volcano (Vanuatu): human and livestock health assessment implications	135
Di Benedetto F., Belluso E., Capella S., Giaccherini A., Romanelli M., Ciuffi B., Montegrossi G., Zoleo A. & Capacci F. - An EPR study of silica radicals in lung tissues with evidence of silicosis.....	136
Fornasaro S., Comodi P., Crispini L., Malatesta C., Zucchini A. & Marescotti P. - Distribution and concentration of potentially toxic elements in ultramafic rocks: a case study from the Voltri Massif (Western Alps, Italy).....	137
Funari V., Toller S. & Costa A. - Human Health vs. Urban Geochemistry during the Anthropic Times	138
Giordani M., Di Lorenzo F., Mattioli M. & Churakov S. - Solubility Assay of the Natural Zeolites Erionite, Offretite and Stellerite	139
Grieco G., Sinojmeri A. & Cavallo A. - Pyrite separation in copper enrichment plants as a key to circular economy driven remediation: a case study from Northern Albania Cu mining district.....	140
Lettino A., Belviso C., Cavalcante F. & Fiore S. - Potential Environmental risk induced by TiO ₂ dispersions in waters and sediments: a case history of the Frido stream deposits (Southern Apennines, Italy).....	141
Mattioli M., Giordani M., Ottaviani M.F., Cangiotti M., Valentini L., Di Giuseppe D. & Gualtieri A.F. - Fibrous ferrierite from the Lessini Mounts, Veneto Volcanic Province, NE Italy.....	142
Medas D., Carlomagno I., Meneghini C., Pusceddu C. & De Giudici G. - Laboratory and synchrotron radiation-based techniques to investigate the soil-plant system in Zn-extreme environments	143
Militello G.M., Gaggero L., La Maestra S., Sanguineti E., Yus González A. & Lavagnino G. - Lower and upper aspect ratio range to consider on quantitative determination of Elongated Mineral Particles (EMP) in bulk samples and in vitro study	144
Moro D., Ulian G. & Valdrè G. - Mechanical properties of calcium apatite-based biominerals: hydroxylapatite (<i>P6₃</i>) and type-A carbonated apatite (<i>PI</i>).....	145
Mousavi Aghdam M., Loi A., Dentoni V., Meloni M.A., Pistis M., Funedda A., Randaccio P. & Da Pelo S. - Can be geogenic radon potential indirectly inferred?.....	146
Parisi F., Sciascia L., Princivalle F., Merli M., Lazzara G. & Milioto S. - Montmorillonite clay for the removal and recovery of metals and dyes from industrial wastewaters	147

Pascucci S., Palombo A., Santini F., Pignatti S., Ionca V., Cavalcante F. & Belviso C. - Hyperspectral thermal data to identify natural and manmade asbestos minerals: TASI-600 imagery case studies	148
Pastero L., Curetti N., Ortenzi M.A., Schiavoni M., Destefanis E. & Pavese A. - Non-conventional CCS reaction: Ca-oxalate precipitation via Vitamin C promoted green reaction	149
Placitu S., Fancello D., Medas D., Alisi C., Paganin P., Tasso F., Sprocati A.R., Turnau K. & De Giudici G. - Mineral dissolution enhanced by bacteria can improve sustainability of agricultural practices	150
Rigonat N., De Giudici G., Medas D., Cidu R., Lattanzi P., Podda F., Dore E., Frau F., Marras P.A. & Frau I. - Assessment of environmental impact of mine drainage on the Rio Montevecchio watershed (SW-Sardinia) through hydrologic-tracer techniques and environmental mineralogy	151
Rizzo G. & Sinisi R. - Mineralogical and petrographical assessment of edenite crystals from Southern Apennine (Italy).....	152
Sacchi E. - Unusual (but not too much) particles in forensic soil samples.....	153
Sacchi E. - Facies analysis at the crime scene: a traditional method in a different frame.....	154
Smiljanić D., Daković A., de Gennaro B., Germinario C., Grifa C., Izzo F., Langella A., Spasojević M. & Mercurio M. - Novel zeolite's nanocomposites with a two-tailed cationic surfactant – Arquad® 2HT-75 with increased stability.....	155
Somma R. - The judicial contribution of the Messina University on Forensic Geology and Environmental Crimes.....	156
Tribaudino M., Mantovani L., Solzi M. & Zaccara P. - Environmental monitoring with magnetic minerals on leaves in wintertime: an assessment.....	157
Valdrè G., Moro D. & Ulian G. - Amino acids-chlorite interaction at the nano-atomic scale.....	158
S5. Geosciences in Archaeometry and Cultural Heritage Conservation	159
Beltrame C., Lazzarini L. & Antonelli F. - The marble identification of ancient shipwrecks for an enhancement of the in situ underwater heritage of Italy: the case of the cargo of Punta del Francese (Stintino-Sassari, Sardinia).....	160
Bernabale M., Nigro L. & De Vito C. - Microstructure and chemical composition of Iron Age archaeological objects from the Phoenician-Punic site of Motya (Sicily, Italy).....	161
Borghi A., d'Atri A., Gambino F., Martire L., Perotti L., Vaggelli G. & Valentino D. - STONE Pietre Egizie: a free mobile application for promoting the knowledge and dissemination of ornamental stones exposed in Museo Egizio of Torino (NW Italy).....	162
Caruso V., Marinoni N., Merlini M., Cantaluppi M., Diella V., Trombino L. & Cattaneo C. - A comparison between the decay of adult and juvenile human skeletons from archeological and contemporary burials using a multidisciplinary approach.....	163
Castagnotto E., Locardi F., Scrivano S., Ferretti M. & Gaggero L. - Chemical and textural fingerprint of natural stones for the use of construction and restoration stakeholders (CatSTONE project).....	164
Coletti C., Maritan L. & Mazzoli C. - “Our Common Future”: a lesson from the past for a renewed responsibility	165
De Francesco A.M., Barca D., Tucci A. & Scarpelli R. - Provenance study of the protohistoric impasto <i>pithoi</i> in the Soverato area (Calabria - Southern Italy) by LA-ICP-MS analysis of individual biotite grains	166
Di Fazio M., Felici A.C., Catalli F., Doménech-Carbó A., Doménech-Carbó M.T. & De Vito C. - Roman orichalcum coins: a deep investigation from patina to core	167
Fioretti G. & Campobasso C. - Petroarchaeometric investigation of building stones and mensiochronological analysis of masonry structures of the St. Maria Veterana archaeological site in Triggiano (Apulia, southern Italy), as multidisciplinary tool for the chronological dating and traditional production technology studies.....	168
Fratini F., Pecchioni E., Cantisani E. & Rescic S. - Pistoia, city of stones.....	169
Germinario C., Cappelletti P., De Bonis A., Di Martire D., Esposito R., Grifa C., Morra V., Rispoli C. & Talamo P. - The Roman villa at the Castle of Baia (Naples, Italy): preliminary investigations on the polychromy of frescoed surfaces by using non-destructive spectroscopic techniques	170

Germinario L. & Oguchi C.T. - Weathering of anthropic caves of soft rock in the Kant? region, Japan.....	171
Giustetto R., Padovan S., Barale L. & Compagnoni R. - The Neolithic <i>greenstone</i> industry from Chiomonte (Turin Province, Northwestern Italy): archaeometric study and comparison with analogous findings ..	172
Manca R., Scrivano S., Manfredi C., Ager Vázquez F. J., Ortega Feliu I., Respaldiza M.A. & Benvenuti M. - Castellani gold jewels: materials characterization by in-situ, non invasive analyses at the Museo di Villa Giulia (Rome)	173
Medeghini L., Botticelli M., De Vito C., Nigro L. & Mignardi S. - Archaeometric analysis on ceramic material from the Khalet al-Jam'a necropolis (Bethlehem, West Bank)	174
Moro D., Ulian G. & Valdrè G. - Monte Carlo SEM-EDS micro- and nanoanalysis in archaeometry and cultural heritage: Thickness, shape/geometry effects and measurement strategy	175
Muntoni I.M., Torre M. & Eramo G. - Setting the technological patterns in the Neolithic pottery production of central Apulia	176
Pancani D., Raneri S. & Gioncada A. - Mineralogical and petrographic evidences of fires at Pisa Cathedral: the case of Panchina Livornese	177
Paris E., Sciarroni G., Virgili S., Abudurehman A. & Antongirolami V. - A newly discovered ceramic production center in Camerino (Marche, Italy)	178
Pellegrini M., Donahue R.E. & Lee-Thorp J.A. - Tracking animal movements with tooth enamel oxygen and strontium isotopes	179
Precisvalle N., Ardit M., Martucci A., Bonadiman C., Bianchini G. & Natali C. - Macedonian ruby: mineralogical and geochemical analysis of a national treasure.....	180
Rispoli C., Cappelletti P., De Bonis A., Di Benedetto C., Esposito R., Graziano S.F., Guarino V. & Morra V. - Historical mortars beyond Pompeii: the example of Villa del Pezzolo (Sorrento Peninsula).....	181
Santi P., Foresta Martin F., Spatafora F., De Vita S., Dell'Aquilano M. & Renzulli A. - Volcanic millstones trade in the Mediterranean during the Hellenistic-Roman period: the impact on the production of manufacts and milling technique evolution at Ustica Island (Southern Tyrrhenian Sea, Italy)	182
Savelli C. - Olduvai Subchron (Pliocene-Pleistocene Transition) In Tyrrhenian Sea and Africa Rift Valley: Geological and Paleoanthropological Implications	183
Scrivano S., Cabella R. & Giannattasio B.M. - Archaeometric contribution to the study of the Small Thermal Baths in the roman town of Nora (Sardinia): mortars and plasters.....	184
Scrivano S., Gambino F., Borghi S., Cabella R. & Giannattasio B.M. - Archaeometric contribution to the study of the Small Thermal Baths in the roman town of Nora (Sardinia): white and coloured marbles	185
Stroscio A., Coccato A., Fugazzotto M., Occhipinti R., Mazzoleni P. & Barone G. - Potentiality of PXRF for the discrimination of altered carbonate rocks in Cultural Heritage.....	186
Testone V., Longo V., Mameli P., Cherchi M. & Milanese M. - Detection of graves and buried walls using ground penetrating radar: the Sant'Antioco di Bisarcio archaeological site (Sardinia).....	187
Tonelli G., Renzulli A., Santi P., Talozzi D., Tramontana M. & Veneri F. - The bricks of the UNESCO historical town of Urbino (Marche, Italy): characterization, provenance of the raw material and archaeometric dating.....	188
Vettori S., Verrucchi M., Di Benedetto F., Gioventù E., Benvenuti M., Pecchioni E., Costagliola P. & Moretti S. - Hyperspectral sensor: a practice tool to evaluate the efficacy of cleaning procedures.....	189
S6. Experimental and theoretical studies of magmatic processes	190
Arzilli F., La Spina G., Burton M.R., Polacci M., Le Gall N., Hartley M., Di Genova D., Cai B., Vo N., Bamber E., Nonni S., Atwood R., Llewellyn E., Heidy M., Brooker R.A. & Lee P. - Highly explosive basaltic eruptions: magma fragmentation induced by rapid crystallisation	191
Buono G., Di Genova D., Fanara S., Palladino D.M., Pappalardo L., Petrosino P., Schmidt B.C. & Sottili G. - The effect of decompression rate and volatile (H ₂ O - CO ₂) content on degassing of trachytic melts ..	192
Buttitta D., Caracausi A., Giannandrea P., Paternoster M., Rizzo A.L. & Rizzo G. - Diffusive fractionation of helium isotopes as a possible process to explain the mantle source feature beneath Mount Vulture volcano (Italy).....	193

Cariddi B., Costamagna L.G., Guarino V., Morra V. & Melluso L. - Petrogenesis of Cenozoic Volcanism in the Cixerri Graben (Southwestern Sardinia)	194
Casiraghi G., Schiavi F., Fumagalli P., Cannaò E. & Tiepolo M. - The effect of chlorine on the incorporation of water in magmatic amphibole in subduction settings: an experimental study at lower crust conditions.....	195
De Cristofaro S.P., Arzilli F., Giordano D., Polo L., Janasi V., Fanara S., Burton M., Polacci M., González-García D. & Masotta M. - Pre- and syn-eruptive conditions of Caxias do Sul silicic magmas (Parana? Magmatic Province, Brazil): Crystallisation kinetics of dacitic melts	196
Di Fiore F., Vona A., Romano C., Sulpizio R. & Mollo S. - The role of undercooling and strain rate on the syn-eruptive rheological evolution of the magma feeding the Pollena eruption of Somma-Vesuvius (Campania; Italy).....	197
Di Genova D. - Volcanic eruptions: a nanoscale perspective	198
Fanara S., Schmidt B.C., Sottili G. & Palladino D.M. - Phase equilibria experiments on a leucitite from the Colli Albani volcanic district (Italy).....	199
Giuliani L., Iezzi G., Davis M., Hippeli T., Vetere F., Elbrecht A.L., Nazzari M., Mollo S. & Scarlato P. - Onset of crystallization in a cooling MORB: an <i>in-situ</i> DSC investigation.....	200
González-García D., Giordano D., Bersani D., Fornasini L., Raneri S., Di Genova D., Dingwell D.B., Russell J.K., Ferrando S. & Lottici P.P. - Raman characterization of natural anhydrous silicate glasses: structure and physical properties of the melt	201
Iacovino K., Giuli G. & Carroll M.R. - Sulfur in alkaline melts: An experimental study.....	202
Milani S., Baratelli L., Comboni D., Maurice J., Lotti P. & Merlini M. - Structure and thermal equation of state of $\text{Ca}_3\text{KNa}(\text{CO}_3)_4$ carbonate	203
Romano P., White J.C., Andujar J., Scaillet B., Di Carlo I., Liotta M. & Rotolo S.G. - Experimental and thermodynamic constraints on mineral equilibria in pantelleritic magmas.....	204
Spartà D., Fumagalli P., Merlini M., Borghini G. & Poli S. - Phase relations in hydrous REE-bearing carbonatite at 1 GPa, 700-1000°C	205
Stabile P., Arzilli F., Paris E. & Carroll M.R. - Role of the kinetics of nucleation and crystal growth of alkali feldspar in a peralkaline pantelleritic melt	206
Stabile P., Appiah H. & Carroll M.R. - Water solubility in Pantelleritic melts.....	207
S7. New frontiers in metamorphism and deformation-metamorphism relationships through cutting-edge analytical, experimental, numerical, and theoretical techniques	208
Angel R.J., Murri M., Prencipe M., Stangarone C., Mihailova B.D. & Alvaro M. - Measuring strains with Raman Spectroscopy	209
Carvalho B.B., Bartoli O., Cesare B., Tacchetto T., Gianola O., Ferri F. & Aradi L.E. - Fate of primary COH fluid inclusions in garnet from high-grade rocks.....	210
Cesare B., Nestola F., Mugnaioli E., Della Ventura G., Peruzzo L., Bartoli O., Viti C., Johnson T. & Erickson T. - I was not born cubic, said low-temperature metamorphic garnet.....	211
Corti L., Visalli R., Zucali M., Mancini L. & Sayab M. - Integrating X-ray microtomography with the chemical imaging of EMPA: A robust method to quantify mineral re-crystallization during metamorphism: example for granulite to eclogite in the Western Alps, Italy	212
Corti L., Zucali M., Delleani F., Zanoni D. & Spalla M.I. - 3D reconstruction of fabric and metamorphic domains in a slice of continental crust involved in the Alpine subduction system: the example of Mt. Mucrone (Sesia-Lanzo Zone, Western Alps).....	213
Croce A., Pigazzi E., Rinaudo C. & Zucali M. - Micro-Raman spectroscopy and microstructural thermometers applied for the evaluation of carbonate mylonites deformation temperature.....	214
Ferrero S., Wannhoff I., Darling R., Wunder B., Laurent O., Ziemann M.A., Günter C. & O'Brien P. - Micropetrology of megagarnets: nanogranitoids reveal presence of melt during formation of the giant garnets of Barton Mine (Adirondacks, US).....	215

Gilio M., Alvaro M., Angel R.J. & Scambelluri M. - Elastic geothermobarometry on multiple inclusions in a single host.....	216
Giuli G., Pratesi G., Radica F., Stabile P., Paris E. & Cibir G. - Iron oxidation state in Fulgurite glass	217
Giuntoli F., Vitale Brovarone A. & Menegon L. - High pressure abiotic methanogenesis and strain localization in metamorphosed carbonate rocks.....	218
Malaspina N., Langenhorst F. & Montanini A. - The oxidation state of C-S-bearing garnet clinopyroxenites from External Liguride (Italy) and Beni Bousera (Morocco): a TEM-EELS study.....	219
Marchesini B., Menegon L., Prando F., Schmidt P.K., Garofalo P.S., Schwarz G., Hattendorf B., Günther D., Mattila J. & Viola G. - Evidence of low-temperature plasticity in naturally deformed pyrite: a LA-ICP-TOFMS-EBSD combined approach (Olkiluoto Island, Finland)	220
Mazzucchelli M.L., Angel R.J., Morganti S. & M. Alvaro M. - EntraPT: a GUI program for anisotropic elastic thermobarometry	221
Menant A., Sternai P. & Gerya T. - Magmatic forcing of Cenozoic climate?.....	222
Mitterpergher S. - From aseismic to seismic slip in exhumed seismogenic sources: insights from geochemical and microstructural studies of pseudotachylyte bearing faults in the Adamello massif	223
Piccoli F., Ague J.J., Chu X. & Vitale Brovarone A. - Multistage metasomatism recorded in HP metamorphic unit: a natural example of porosity waves in subduction zones?	224
Schwarzenbach E.M., Li J., John T., Caddick M.J., Petroff M. & Gill B.C. - Sulfur transfer within subduction zones: Evidence from exhumed mafic and ultramafic slab material.....	225
S8. Permo-Triassic geodynamic evolution of the Western Tethys realm: insights from magmatism, tectonics and stratigraphic data	226
Brack P. - Timing of Middle Triassic Magmatism in the Southern Alps.....	227
Brombin V., Bonadiman C., Jourdan F., Roghi G., Coltorti M., Webb L.W., Callegaro S., Bellieni G., De Vecchi Gp., Sedeo R. & Marzoli A. - Deciphering a geological enigma: occurrence of intraplate magmatism at convergent plate boundaries.....	228
Caggiati M. & Gianolla P. - Distribution of Triassic magmatism in the Southern Alps: an updated overview .	230
Casetta F., Ickert R.B., Mark D.F., Bonadiman C., Giacomoni P.P., Ntaflou T. & Coltorti M. - The alkaline-carbonatitic lamprophyres of the Dolomitic Area: Late Triassic precursors of the Alpine Tethys opening	231
Casetta F., Giacomoni P.P., Nardini N. & Coltorti M. - Petrological features of clinopyroxene in lava flows from Cima Pape (Dolomitic Area, Southern Alps): how to unravel the feeding system of a Middle Triassic volcano	232
Curzi M., Gianolla P., Caggiati M. & Carminati E. - Middle Triassic subsidence in the Dolomites (Italy): control of tectonics	233
Ferrari E., Tribuzio R., Bosch D., Bruguier O. & Langone A. - Lower Carboniferous to Upper Triassic evolution of the Ivrea-Verbano Zone: geochronological constraints from the Alpe Morello (Val Strona) rock sequence.....	234
Martin S., Toffolo L., Moroni M., Montorfano C., Secco L., Agnini C., Nimis P. & Tumiatì S. - Early Permian - Early Triassic siderite deposits in the Southern Alps (Italy).....	235
Mazzucchelli M., Giovanardi T. & Cipriani A. - Mantle carbonatites or anatectic carbonatites of crustal origin in the Ivrea-Verbano Zone?.....	236
Molli G., Brogi A., Caggianelli A., Capezzuoli E., Liotta D., Spina A. & Zibra I. - A review of upper Carboniferous-Permian tectonics in Corsica, Calabria and Tuscany	237
Morelli C., Bargossi G.M., Gasparotto G., Mair V., Moretti A., Piccin G. & Trentini T. - Outline of a mega volcanic system: The Athesian Volcanic Group	238
Pecorari M., Gianolla P. & Caggiati M. - The onset of Middle Triassic volcanism in the Dolomites (Southern Alps, Italy)	239
Roda M., Regorda A., Spalla M.I. & Marotta A.M. - What drives Alpine Tethys opening? Clues from the review of geological data and model predictions	240

Succo A., Festa A., Balestro G., Borghi A. & De Caroli S. - Role of Late Carboniferous - Early Triassic structural inheritance in the continental break-up of Pangea and exhumation of the Alpine Tethyan mantle: insights from the Canavese Zone, Western Alps	241
Velicogna M., Venier M., Brombin V. & De Min A. - Comparison among the volcanic complex of Gorski Kotar and lava flows from the Medvednica Mountains with the Triassic magmatism of the Dolomites, first results	242
Zanetti A., Giovanardi T., Morishita T., Hemond C., Dallai L., Langone A. & Mazzucchelli M. - Evidence for subduction-related components in sapphirine-bearing gabbroic dykes (Finero Phlogopite peridotite): Insights into the mantle sources of the Mesozoic magmatism at the Africa-Europe boundary	243
S9. Isotopic tracers and timing of dynamic evolution of subduction zone settings	244
Agostini S., Di Giuseppe P., Manetti P., Savascini M.Y., Doglioni C. & Conticelli S. - Early Miocene to Pleistocene Na-alkaline Volcanism on the North-East Arabian plate (South-East Turkey)	245
Bragagni A., Mastroianni F., Avanzinelli R., Conticelli S. & Münker C. - Extreme HFSE fractionation in Italian magmas: metasomatism vs. different mantle domains.....	246
Cannaò E., Scambelluri M. & Tiepolo M. - Into deep and beyond: carbon and nitrogen subduction recycling by secondary peridotites	247
Cannaò E., Tiepolo M., Sessa G., Deloule E. & Poli S. - Amphibole as carbon fixing mineral at lower crust depth	248
Casalini M., Avanzinelli R., Tommasini S., Garzonio C.A., Cioni R. & Conticelli S. - Genesis and differentiation of a calc-alkaline volcano in syn-collisional continental setting: the Mount Ararat (A?r? Da??, Eastern Anatolia)	249
Di Giuseppe P., Agostini S., Manetti P., Savascini M.Y. & Conticelli S. - Early Miocene to Pliocene magmatic activity in the Sivas-Malatya Volcanic Region (Central-Eastern Anatolia)	250
Elliott T., Freymuth H., Andersen M., Chen S. & Hin R. - Isotopic fractionations between dehydration fluid and descending slab	251
Gilio M., Scambelluri M., Agostini S., Godard M., Pettke T., Agard P., Locatelli M. & Angiboust S. - Fingerprinting and relocating tectonic slices along the plate interface: evidence from the Lago Superiore Unit at Monviso (Western Alps)	252
Malaspina N. & Tumiati S. - Redox processes and the role of carbon-bearing volatiles at subduction zones: natural versus experimental perspectives	253
Narduzzi F., Farina F., Lana C., Teixeira L., Schannor M., Stevens G., Alkmim A. & Nalini Jr H.A. - Long-lived petrological cannibalism and slow cooling rates for the Galiléia batholith (SE Brazil): supporting the “hot” nature of Araçuaí-West Congo orogen.....	254
Natali C., Aghazadeh M., Braschi E., Badrzadeh Z., Bianchini G. & Conticelli S. - Eocene subduction to collision-related volcanism in the Arasbaran area (NW, Iran): evidence for progressive evolution of mantle sources	255
Tamburello G. - The importance of direct gas flux measurements at active volcanoes for understanding the geochemical cycles in the subduction zones	256
Tumiati S. - Dissolution of graphite in high-pressure aqueous fluids: the roles of crystallinity and of coexisting silicates and carbonates	257
Tumiati S. - Decoupling between the carbon isotopic signature of CO ₂ -bearing aqueous fluids and of their graphite+carbonate source at subarc depth.....	258
S10. Metasomatic and refertilization processes in lithospheric mantle: unraveling the heterogeneities in mantle sources and related geodynamic systems	259
Alipour R., Perinelli C., Moeinzadeh H., Ahmadipour H., Bosi F. & Gaeta M. - Mineralogical and petrogenetic characteristics of the peridotites and associated podiform chromitites from Abgarm ultramafic complex (south-eastern Iran).....	260

Andreozi G.B., Bosi F., Conte A.M., Cuccuru S. & Naitza S. - Evaluating the controls on the origin of tourmaline-bearing rocks in peraluminous and metaluminous systems: examples from Late-Variscan magmatism of Sardinia (Italy).....	261
Antonicevich M., Tribuzio R., Wu F.Y. & Liu T. - Origin of the peridotite-pyroxenite association from Rocca di Argimonia, Ivrea Mafic Complex (Ivrea-Verbanò Zone).....	262
Bonadiman C., Pelorosso B., Curetti N., Merli M., Coltorti M. & Pavese A. - Phlogopite-pargasite coexistence in spinel peridotite xenoliths from Mount Leura (southeast Australia).....	263
Borghini G., Fumagalli P. & Rampone E. - Peridotite modification via reaction with pyroxenite-derived andesitic melts: an experimental study at 2 GPa.....	264
Casetta F., Giacomoni P.P., Ferlito C., Bonadiman C. & Coltorti M. - From the 600 ka tholeiites to the recent trachybasaltic magmas at Mt. Etna: evolution of a lherzolitic mantle.....	265
Consuma G., Braga R., Giovanardi T., Bersani D., Konzett J., Lugli F., Mazzucchelli M. & Tropper P. - The Carbon pathway through subduction zones: petrological and geochemical constraints on carbonates from garnet-bearing orogenic peridotites.....	266
Conte A.M., Perinelli C., Bigi S., Bosman A., Castorina F., Conti A., Cuffaro M., Di Vincenzo G. & Martorelli E. - New insights on volcanic activity related to the opening of the Central Tyrrhenian Sea: the transitional basalts of the Ventotene Volcanic Ridge (Pontine Islands, Italy).....	267
Correale A., Pelorosso B., Rizzo A.L., Coltorti M., Italiano F., Bonadiman C. & Giacomoni P.P. - The noble gases geochemistry in mantle xenoliths from West Antarctic Rift System.....	268
Faccini B., Coltorti M., Brenna M., Casetta F. & Briggs R. - Multiple subduction-related metasomatic pulses in mantle xenoliths from the Karioi volcano, North Island, New Zealand.....	269
Fumagalli P., Borghini G., Klemme S. & Rampone E. - Major and trace elements distribution during high-pressure melt-peridotite reaction: experiments at 2 GPa.....	270
Giacomoni P.P., Coltorti M., Bonadiman C., Ferlito C., Faccini B., Zanetti A. & Ottolini L. - From mantle to magma: a volatile budget between mantle xenoliths and primary magmas in the Western Antarctic Rift System.....	271
Giovanardi T., Girardi V.A.V., Teixeira W., Mazzucchelli M. & Cipriani A. - Mafic dyke swarms at 1882, 535 and 200 Ma in the Carajás region: an insight on the evolution of the sub- Amazonian Craton mantle.....	272
Giovanardi T., Zanetti A., Langone A., Cipriani A. & Mazzucchelli M. - Dioritic-albititic dykes in the Finero Phlogopite Peridotite: an intrusive event in the Northern Ivrea-Verbanò Zone (Southern Alps).....	273
Mazzucchelli M., Bertotto G.W., Giovanardi T., Zanetti A., Ponce A.D., Brunelli D., Bernardi M.I., Hémond C. & Cipriani A. - Xenoliths's evidence for refertilisation of a strongly depleted mantle column in the Patagonian extra-Andean backarc (Paso de Indios, Argentina).....	274
Pellegrino L., Malaspina N., Zanchetta S., Langone A. & Tumiati S. - Eclogite-derived melts-peridotite interaction at HP in the Monte Duria area (Central Alps, N Italy): a proxy for the mafic crust-to-mantle mass transfer in subduction zones.....	275
Rizzo A.L., Coltorti M., Faccini B., Casetta F., Ntaflou T. & Italiano F. - Petrological features and volatile content of ultramafic xenoliths from Eifel (Germany).....	276
Salari G., Rahimzadeh B., Agostini S., Masoudi F. & Lustrino M. - Quaternary ultrabasic volcanic rocks in central Urumieh-Dohkhtar magmatic arc (Central-Northern Iran): melanephelinites in post-collisional setting.....	277
Venier M., Bernardini F., Caldeira R., de Ignacio C., Marzoli A., Mata J., Princivalle F., Boumehdi M.A., Bensaid I.A.A., Youbi N., De Min A. & Lenaz D. - MicroCT rendering of spinel-facies mantle xenoliths.....	278
S11. Mantle Petrology: from observation to calculus.....	279
Belmonte D. - <i>Ab initio</i> thermodynamics of deep mantle phase transitions and seismic discontinuities: the role of MgSiO ₃ polymorphs.....	280
Del Vecchio A., Poe B.T., Cestelli-Guidi M. & Misiti V. - Point defect equilibria in hydrous forsterite synthesized at 1100°C and up to 4 GPa.....	281

Li P., Xia Q.-K., Dallai L., Bonatti E., Brunelli D., Cipriani A. & Ligi M. - H ₂ O Enrichment in Residual Mantle Peridotites at a Mid-Atlantic Ridge Segment.....	282
Merli M., Bonadiman C. & Pavese A. - Earth's non-primitive lower mantle: aluminium recycling	283
Merli M., Bonadiman C. & Pavese A. - Oxidation state of iron in the Earth's lower mantle	284
Moretti R. - Vapor-buffered magmatic activity and the unique CO ₂ -rich source of magmatism in Southern Italy.....	285
Ottonello G., Belmonte D. & Vetuschi Zuccolini M. - Thermochemistry of silicate melts in high-rank simplexes: the new HPA model	286
Papale P. - Why do we need mathematical models in petrology and volcanology?.....	287
Sanfilippo A., Sokolov S., Salters V.J.M., Stracke A. & Peyve A. - Melting an anciently depleted mantle	288
Vetuschi Zuccolini M., Ottonello G. & Belmonte D. - TRIangular DIagram and deSCENT line analysis - a code to generate a computationally manageable liquidus surface of a molten silicate system and a consistent cooling descent line description from modelling	289
S12. Advances in Understanding Geological and Petrological Processes in the Oceanic Lithosphere..	290
Assanelli M., Luoni P., Rebay G. & Spalla M.I. - Structural and metamorphic evolution of Gias Vej serpentinites (Piemonte Zone, Lanzo Valley, Italian Western Alps).....	291
Basch V., Rampone E., Ferrando C., Borghini G. & Zanetti A. - pMELTS modeling of depleted melts evolution in oceanic environment: implications of pyroxenite formation as deep melt segregation	292
Bonatti E. Early days of the plate tectonics revolution - "Geo-data gatherers" versus "Geopoets".....	293
Borghini G. & Fumagalli P - Partial melting experiments on olivine-free pyroxenites at 2 GPa	294
Brunelli D., Maia M., Ligi M., Bonatti E., Briais A., Campos T., Ceuleneer G., Cipriani A., Cuffaro M., Gregory E., Hamelin C., Jbara R., Kaczmarek M.-A., Lombardi F., Moreira S., Mougél B., Petracchini L., Puzenat V., Revillon S., Seyler M., Soltanmohammadi A., Verhoest L., Trivellato T. & Wang Z. - Cold spots at Mid Ocean Ridges help revealing mantle heterogeneity: a summary of the SMARTIES cruise in the Equatorial Atlantic.....	295
Deraco M., Sanfilippo A., Ligi M., Rasul N., Vigliotti L., Jerais A., Tharowi A., Langone A. & Zanetti A. - Formation of a hybrid oceanic crust at the onset of the Red Sea opening (Tihama Asir magmatic complex; Saudi Arabia).....	296
Ferrari E., Montanini A., Secchiari A., Bosch D. & Cluzel D. - Pyroxenite diversity in the New Caledonia mantle sequence: a preliminary study	297
Grammatica M., Fumagalli P. & Borghini G. - The role of melt/rock ratio in olivine-rich troctolite formation via basalt-dunite reaction: an experimental study at 0.5 GPa.....	298
Guerini S. & Tartarotti P. - Listvenites in the western Alps: the case of the Mount Avic massif (Aosta Valley, northwestern Alps).....	299
La Rosa A., Pagli C., Keir D., Sani F., Corti G., Wang H. & Posee D. - Observing oblique slip during rift-linkage processes in Northern Afar	300
Ligi M., Bonatti E., Brunelli D. & Cuffaro M. - Global Seafloor Spreading Variations and the Evolution of Seawater Composition since the Mesozoic	301
Luoni P., Rebay G., Roda M., Spalla M.I. & Zanoni D. - UHP relics in the Zermatt-Saas Zone serpentinites: new puzzle tiles in the geodynamic scenario.....	302
Maino M., Casini L., Sanfilippo A. & Ildefonse B. - From dislocation creep to grain boundary sliding in high-temperature troctolites: insights into shear localization mechanisms in the oceanic crust.....	303
Montanini A., Secchiari A., Bosch D. & Tribuzio R. - Pb isotope composition of recycled mantle pyroxenites: insights into the the HIMU source of oceanic basalts?.....	304
Mosconi A., Sanfilippo A., Liu C.Z., Salters V., Tribuzio R. & Zanetti A. - Isotopic heterogeneity of mantle melts migrating through the Lanzo South Ophiolite: a focus on Re-Os isotopes and PGE.....	305
Renna M.R., Tribuzio R., Sanfilippo A., Armandola S., Becker H. & Wang Z. - Highly siderophile elements and Re-Os isotopes of primitive oceanic troctolites: implications for reactive processes during lower crust formation.....	306

Salvioli-Mariani E., Boschetti T., Toscani L., Montanini A., Petriglieri J.R. & Bersani D. - Multi-stage rodingitization of ophiolitic bodies from Northern Apennines (Italy): constraints from petrography, geochemistry and thermodynamic modelling.....	307
Sani C., Sanfilippo A., Ohara Y., Snow J., Harigane Y. & Yamahshita H. - Mado Megamullion (Shikoku basin): a new window into a backarc lower crust and mantle.....	308
Sani F., Bonini M., Corti G. & Moratti G. - The role of rift width in controlling fault pattern and kinematics in oceanic and continental rifts: examples from Iceland and Ethiopia.....	309
Savelli C. - Oceanization and Hydrography (West Mediterranean)	310
Sternai P. - Surface processes forcing on rift magmatism: insights from numerical modeling.....	311
Verhoest L., Brunelli D., Hemond C., Bonatti E., Ligi M. & Cipriani A. - Mantle source heterogeneity in the Equatorial Mid Atlantic Ridge: a multi-isotopic approach.....	312
S13. A multidisciplinary approach to unravel the evolution of basement geology	313
Bartoli O. - Constraining fluid regime during melting of crystalline basements: experiments vs. thermodynamic modelling.....	314
Benà E., Martin S., Marzoli A., Mazzoli C., Sassi R. & Zattin M. - Apatite (U-Th)/He thermochronometry from trachytes and latites of the Euganean Hills and their exhumation history.....	315
Bonazzi M., Langone A., Zanetti A., Dellarole E., Mazzucchelli M. & Giovanardi T. - Origin of Plumasite dykes intruded in Variscan basement during triassic: new insights from Zircon (Val Sabbiola, Ivrea-Verbano zone).....	316
Carosi R., Montomoli C., Iaccarino S. & Visonà D. - The High Himalayan Discontinuity and the Main Central Thrust in Central Nepal: timing constraints by in-situ U-Th-Pb monazite petrochronology	317
Carosi R. - Partitioned transpressional tectonics in the Variscan Basement of northern Sardinia (Italy).....	318
Casini L., Corvo' S., Maino M., Seno S. & Schenker F. - Numerical modelling of floating P-T conditions in inclusion-matrix systems, with application to the Cima Lunga Unit (Central Alps)	319
Corvo' S., Maino M., Langone A., Piazzolo S., Seno S. & Schenker F. - Determination of P-T-t-d path in a high-grade shear zone: petro-chronological and microstructural study from the Cima di Gagnone (Adula-Cima Lunga nappe, Central Alps).....	320
Cruciani G., Franceschelli M., Massonne H.-J. & Musumeci G. - P-T path of felsic granulite from south-east Corsica (France) and implications for geodynamic setting.....	321
Franceschelli M. & Cruciani G. - Clockwise and anticlockwise P-T path in the axial zone of the Variscan Sardinia-Corsica block	322
Giuntoli F., Menegon L., Warren C., Darling J. & Anderson M. - Protracted shearing at mid crustal conditions in the Scandinavian Caledonides	323
Iaccarino S., Carosi R., Montomoli C., Montemagni C., Massonne H.-J., Jain A.K. & Visonà D. - Geology and tectono-metamorphic history of the Himalayan metamorphic core: insights from the Alaknanda-Dhauli Ganga valleys (NW India).....	324
Möller C., Andersson J. & Rebay G. - High-temperature metamorphism and deformation in the footwall of an eclogite-bearing nappe, Sveconorwegian orogen: metamorphic evolution of the Obbhult Complex, SW Sweden	325
Martini M. & Zepeda-Martínez M. - The Jurassic exhumation history of basement rocks in Mexico preserved in the stratigraphic record of rift basins associated to Pangea breakup	326
Molli G., Vitale Brovarone A., Beyssac O. & Cinquini I. - Thermal architecture and deformation structures in the Alpi Apuane (NW Tuscany Italy): new insights for the metamorphic and tectonic history of the inner northern Apennines.....	327
Montemagni C., Zanchetta S., Montomoli C., Iaccarino S., Visonà D., Villa I.M. & Carosi R. - Geochronology and kinematics of flow of the Main Central Thrust zone in the Bhagirathi valley, NW Indian Himalaya	328
Morelli G., Ruggieri G., Zucchi M., Braschi E., Agostini S., Ventruti G., Brogi A., Liotta D., Boschi C. & González-Partida E. - Characterization and evolution of the paleo-fluids in the Las Minas exhumed geothermal system (Mexico)	329

Nania L., Montomoli C., Iaccarino S., Leiss B., Di Vincenzo G. & Carosi R. - Kinematics and deformation temperatures of the MCTz and the STDS in Central Himalaya	330
Ortolano G., D'Agostino G., Visalli R., Fiannacca P. & Cirrincione R. - Development of vermicular clinopyroxene-amphibole symplectites replacing garnet in amphibolites of the Peloritani Mountain (Northeastern Sicily).....	331
Ortolano G., Visalli R., Fazio E., Fiannacca P., Godard G., Pezzino A., Punturo P., Sacco V. & Cirrincione R. - Unravelling cooling rates of the Calabria continental lower crust from combined microstructural, thermodynamic and diffusion modeling: An example from the Sila Piccola Massif, (Northern Calabria)	332
Petroccia A., Carosi R., Montomoli C. & Simonetti M. - Geochronology and deformation in the Posada-Asinara Line (NE Sardinia basement, Baronia, Italy): timing and shearing constraints in the Southern European Variscan belt	333
Petroccia A., Carosi R., Montomoli C. & Simonetti M. - 1:25.000 structural map of Mamone in the northern of the Sardinian variscan basement	334
Renna M.R., Langone A., Caggianelli A. & Prosser G. - Interaction between migmatite-related melts and amphibole-gabbros: evidence from mineral geochemistry and zircon dating (Variscan lower crust, Palmi area, SW Calabria)	335
Simonetti M., Carosi R. & Montomoli C. - Extension, timing and deformation of the East Variscan Shear Zone	336
Simonetti M., Carosi R. & Montomoli C. - Structural analysis, kinematic of the flow and petrochronology of shear deformation in the Aiguilles Rouges Massif.....	337
Tursi F., Acquafredda P., Festa F., Fornelli A., Langone A., Micheletti F. & Spiess R. - Reworking of felsic rocks in ductile shear zones: an example from the Curinga-Girifalco line.....	338
Van Schroyen Lantman H.W., Langone A., Scambelluri M. & Alvaro M. - Uncovering UHPM garnet growth and dissolution mechanisms using trace elements in metasediments from Lago di Cignana, Western Alps.....	339
Zepeda-Martínez M. & Martini M. - Tectono-sedimentary evolution of the Tlaxiaco Basin, southern Mexico: A key to understand the Jurassic structural history of Proterozoic and Paleozoic basement rocks of Mexico during Pangea breakup.....	340
Zucchi M. - Faults-controlling geothermal fluid flow in low permeability rock volumes: an example from the eastern Elba Island (northern Tyrrhenian Sea, Italy).....	341
S14. Bio-Geo materials for environmental remediation: novel approaches, technologies and case studies	342
Artioli G., Berto D., Dalconi M.C., Gò E., Peruzzo L. & Tateo F. - Occurrence of pararealgam in As-rich aquifer sediments of the Venetian plain (Italy).....	343
Deltedesco E., Zehetner F., Unterfrauner H. & Keiblinger K.M. - Microbiological assessment of lime application to agricultural soils.....	344
Faccini B., Di Giuseppe D., Ferretti G., Galamini G. & Coltorti M. - Effects of natural and NH ₄ -enriched Zeolite on nitrogen leaching from a reclaimed agricultural soil of the Ferrara province (Italy)	345
Ferretti G., Galamini G., Deltedesco E., Gorfer M., Faccini B., Zechmeister-Boltenstern S., Coltorti M. & Keiblinger K.M. - Effects of natural and NH ₄ -charged zeolite amendments and their combination with 3,4-dimethylpyrazole phosphate (DMPP) on soil gross ammonification and nitrification rates.....	346
Ferretti G., Keiblinger K.M., Faccini B., Galamini G., Mentler A., Zechmeister-Boltenstern S. & Coltorti M. - Sorption of 3,4-Dimethylpyrazole phosphate (DMPP) in Soils amended with different chabazite zeolites.....	347
Keiblinger K.M., Maftukhah R., Ngadisih, Murtiningrum, Kral R.M. & Mentler A. - Soil amendments for re-cultivation of formerly mined land on Bangka island, Indonesia	348
Leoncini C., Lo Monaco A., Gagni S., Emiliani R., Riberti R., Forti F., Caridei F., Filippini M. & Gargini A. - Optimal hydrogeological conditions for phytoscreening in sites with chloroethenes subsurface contaminations.....	349

Malferrari D., Bernini F., Bigli B., Borsari M., Brigatti M.F., Castellini E., Mucci A. & Sebastianelli L. - Sulfur bearing and aromatic compound trapping by layered silicates: a great start for innovative technological applications	350
Matteucci F., Curri M.L., Comparelli R., Giannantonio R., Giansante C., Mascolo G. & Giannini C. - Nanomaterials for the abatement of contaminants in water treatment	351
Mentler A., Ottner F., Wriessnig K., Keiblinger K.M. & Kral R.M. - Production potential in central Mozambique: soil analysis and mineralogy	352
Mentler A., Keiblinger K.M., Maftukhah R., Ngadisih N., Murtiningrum M. & Kral R.M. - On the ground or in the ground? Co-learning of farmers and scientists about soil	353
Molinari S., Salviulo G., Magro M., Baratella D. & Vianello F. - Water total arsenic remediation via a new generation colloidal superparamagnetic maghemite nanoparticles	354
Morrone L., Facini O., Mari M. & Rotondi A. - Effects of zeolite and kaolin foliar application in olive trees on photosynthesis and on drupes oil content	355
Morrone L., Mari M. & Rotondi A. - Use of geo materials (zeolites) in the rooting phase for the production of olive plant	356
Neri L., Carriero G., Facini O. & Baraldi R. - Environmental remediation of the historical suburban forest Bosco Albergati	357
Neri L., Monti A. L., Ottoni S., Facini O. & Baraldi R. - Phytoremediation of contaminated sites: the case study of a petroleum refinery in Mantova, Italy	358
Prisa D. - Chabazitic-zeolites and Effective Microorganisms for the qualitative improvement and fertilizers reduction in the growth of Aloe plants	359
Prisa D. - Improvement Quality and Content of Pepper and Chilli Nitrates Influenced by the Effective Microorganisms	360
Rizzo P., Sanangelantoni A., Iacumin P. & Celico F. - Isolation and selection of bacterial strains for aquifer remediation: a case study in Val d'Agri (Southern Italy)	361
S15. Geobiology: Biosphere-Earth interactions	362
Azzarone M., Cheli A., Mancuso A., Stagioni M., Falini G., Goffredo S. & Scarponi D. - <i>Chamelea</i> <i>gallina</i> response to a warming Earth: A case study from the Holocene sedimentary succession of the Po-Adriatic system	363
Berton D., Rodriguez Navarro A., Grenier Romero C., Roman Martinez R., Rodeghero E. & Martucci A. - The precipitation process of the calcium carbonate in <i>Austrorhynchus Psittacus</i> and the role of organic matter: a multidisciplinary study	364
Bonacina G., Sanfilippo A., Previde Massara E., Scotti P., Viaggi P. & Piva A. - The Cretaceous Oceanic Anoxic Event 2: geochemical constraints from a section of the Atlantic margin	365
Bosio G., Bracchi V.A., Malinverno E., Basso D., Collareta A., Gioncada A., Coletti G., Di Celma C. & Bianucci G. - Taphonomic and diagenetic history of a Panopea-rich layer from the Pisco Formation, Peru	366
Bracchi V.A. & Basso D. - Crustose coralline algae: the bioengineers of Mediterranean seafloor at the geological scale	367
Bragato P.L. - Human and geological crises of the last millennium in Italy modulated by the episodes of the Little Ice Age	368
Consani S., Borello A., Vezzulli L. & Carbone C. - Characterisation of prokaryotes and eukaryotes in contaminated extreme environments: preliminary results	369
Leonelli G., Pelfini M. & Maggi V. - Changes in the tree-ring $\delta^{18}\text{O}$ from the Forni Glacier forefield due to glacier stream water inputs and climate change: potential use for environmental and climatic reconstructions	370
Malferrari D., Ferretti A., Mascia M.T., Medici L. & Savioli M. - Integrated strategies for quantifying major element contents in modern and fossil bioapatite	371
Notaro A., Garzarella A. & Raffi I. - Calcareous nannofossils behavior during global warmth intervals of the Neogene	372

Vertino A., Savini A. & Marchese F. - Bio-geosphere interactions in the deep: The important role of cold-water corals.....	373
S16. Planetary evolution: new insights from remote sensing, in-situ, terrestrial analogues and meteorite studies	374
Antonangeli D., Badro J., Boccato S., Morard G., Rivoldini A., Siebert J., Xu F. & the InSight Science Team - InSight, first months on Mars and laboratory experiments to complement planetary observations.....	375
Baioni D., Gutierrez F., García-Arnay A., Luzzi E., Parenti C., Sevil J. & Nesci O. - Two possible episodes of karstification in the equatorial layered deposit within Kotido crater, Arabia Terra, Mars	376
Campanale F., Mugnaioli E., Folco L., Gemmi M., Lee M.R., Daly L. & Glass B.P. - Evidence for direct solid-state quartz-to-coesite transformation in shocked ejecta from the Australasian tektite/microtektite strewn field	377
Carli C., Morlok A., Stojic A., Weber I., Renggli C., Klemme S., Ferrari S., Pratesi G., Hiesinger H. & Capaccioni F. - VNIR reflectance spectra of iron-bearing Mercury-like glasses	378
Fastelli M., Comodi P., Zucchini A., Maturilli A., Balic-Zunic T. & Rossi M. - Reflectance and emissivity spectroscopy of hydrated salts at different temperature: a method to understand icy planetary bodies surfaces composition	379
Folco L. - The near-Earth cosmic dust complex: Perspectives from the unique Transantarctic Mountains micrometeorite collection	380
Galluzzi V., Ferranti F., Massironi M., Giacomini L., Guzzetta L. & Pasquale P. - High-Mg region induced stress field in the Victoria quadrangle of Mercury.....	381
Giacomini L., Galluzzi V., Carli C., Zambon F., Massironi M., Ferranti L. & Palumbo P. - Geological mapping of the Kuiper (H06) quadrangle of Mercury: Integration between morphologic and spectral characteristics	382
Italiano F., Di Bella M., Sabatino G., Barbieri R., Cavalazzi B., Ferretti A., Danovaro R., Romeo T., Andaloro F., Esposito V., Tripodo A., Scotti G. & Quartieri S. - Hydrothermal iron ooids on Earth as homologues of hematite spherules discovered on Mars.....	383
Massironi M., Pozzobon R., Franceschi M. & Penasa L. - From Planetary surface mapping to Planetary subsurface structures.....	384
Miozzi F., Morard G., Antonangeli D., Clark A.N., Baron M.A., Dorn C., Rozel A., Pakhomova A., Mezouar M. & Fiquet G. - Characterization of the Fe-Si-C system at extreme conditions and application to exoplanets interior	386
Moggi Cecchi V., Pratesi G., Giuli G., Nemati M., Di Martino M. & Serra R. - The 2017 Joint Italian - Iranian Lut desert expedition: compositional and textural features of the meteorites recovered.....	387
Mugnaioli E., Gemmi M., Campanale F., Suttle M.D., Folco L. & Pignatelli I. - 3D electron diffraction for the characterization of cryptocrystalline micro-samples: Applications to planetary sciences	388
Nava J., Maturilli A., Zambon F., Carli C., Alemanno G., Helbert J., Genovesi S. & Massironi M. - Laboratory experiments on carbonaceous chondrites: insights into cryovolcanism and hydrothermal alteration on planetary bodies.....	389
Nazzareni S., Pauselli C., Skogby H., Murri M., Domeneghetti M.C., Alvaro M., Stalder R., Petrelli M., De Sanctis M.C., Formisano M. & Federico C. - Pyroxenes as a proxy for thermal history and water content of asteroid 4 Vesta.....	390
Nestola F., Barbaro A., Morana M., Christ O., Brenker F.E., Domeneghetti M.C., Dalconi M.C., Alvaro M., Goodrich C., Fioretti A.M., Leoni M. & Shaddad M.H. - Diamonds in ureilites: how did they form?..	391
Pisello A., De Angelis S., Ferrari M., Vetere F.P., Pauselli C., Kueppers U., De Sanctis M.C. & Perugini D. - A new spectroscopic database for silicate glasses: implications for planetary science.....	392
Re C., Cremonese G., Naletto G. & Tordi M. - HYPSON, Next generation of a stereo camera	393
Suttle M.D., Twegar K., Nava J., Spiess R., Spratt J., Campanale F. & Folco L. - A unique CO-like micrometeorite hosting an exotic Al-Cu-Fe-bearing assemblage – close affinities with the Khatyrka meteorite	394

Tangari A.C., Marinangeli L., Scarciglia F., Pompilio L. & Piluso E. - Genesis and age of clay deposits in Margaritifer Region on Mars using terrestrial soil analogues	395
Tribaudino M., Mantovani L., Bersani D. & Salviati G. - Cathodoluminescence and photoluminescence: combined SEM-EDS and Raman to approach the analysis of anorthite in Ca-Al inclusions	396
Zambon F., Carli C., van der Bogert C.H., Hiesinger H., Altieri F., Giacomini L. & Massironi M. - Spectral variations across Apollo basin on the Moon.....	397
S17. Unveiling the Antarctica: geological, geophysical and sedimentological approaches to the evolution of Antarctica	398
Balestrieri M.L., Olivetti V., Rossetti F., Gautheron C. & Zattin M. - Topography, structural and thermochronological analysis in the Admiralty Block, northern Victoria Land, Antarctica: decoding the Cenozoic evolution of the NE termination of the Transantarctic Mountains	399
Battaglia F., Baradello L., De Santis L., Gordini E., Sauli C., Kovacevic V., Morelli D., Langone L., Colleoni F., Colizza E., Rebesco M. & Accetella D. - High resolution seismo-stratigraphic evidence from the Edisto Inlet fjord, western Ross Sea (Antarctica).....	400
Capponi G., Montomoli C., Casale S., Simonetti M., Musumeci G. & Salvatore M.C. - Geology of the Convoy Range and Franklin Island quadrangle, Victoria Land - Antarctica.....	401
Cornamusini G., Zurli L., Perotti M. & Talarico F.M. - Deformational structures in Paleozoic sandstones of the Transantarctic Mountains: glacial vs tectonic origin	402
Dal Seno N., Lelli L., Millikin L., Smith Lyttle B., Cox S.C., Crispini L. & Burton-Johnson A. - GeoMAP dataset of the Antarctic Peninsula.....	403
Dallai L. & Sharp Z.D. - Continental hydrology and atmospheric circulation during Cenozoic super warm periods	404
De Santis L., Olivo E., Sorlien C., Kim S., Granot R., Sauli C., Busetti N., Wardell N., Rui L., Perez L.F., Colleoni F., Pochini E., Wilson D., Bart O.J., McKay R.M., Kulhanek D. & IODP Expedition Scientific Party - Miocene paleobathymetric reconstruction of the Ross Sea (Antarctica)	405
Federico L., Cianfarra P., Crispini L., Capponi G., Rossi C. & Salvini F. - Reconstruction of multiple tectonic events in the Rennick Geodynamic Belt (northern Victoria Land, Antarctica) through inversion of fault slip data	406
Ferraccioli F., Armadillo E., Crispini L., Läufer A., Ruppel A. & Lisker F. - Crustal architecture of a major pull apart basin in northern Victoria Land, East Antarctica.....	407
Ferraccioli F., Jordan T.A., Forsberg R., Eagles G., Eglington B., Kuszniir N., Olesen A., Matsuoka K., Casal T. & Paxman G. - Aerogeophysical imaging unveils the architecture and basement of the Pensacola-Pole subglacial basin in East Antarctica.....	408
Giacomoni P.P., Coltorti M., Bonadiman C., Ferlito C., Casetta F., Zanetti A. & Ottolini L. - Subduction-related volatiles involved in the genesis of Cenozoic primary alkaline melts in Northern Victoria Land.....	409
Guzzo G., Cattò S., Olivetti V., Zattin M., Balsamo F., Balestrieri M.L. & Rossetti F. - Thermochronological evolution of Transantarctic Mountains in the Mt Murray area.....	410
Iaccarino S., Carosi R., Montomoli C. & Massonne H.-J. - Tectonometamorphic evolution of the Dessent Unit (northern Victoria Land, Antarctica): new data from pseudosection modeling of metasediments .	411
Li X., Zattin M. & Olivetti V. - The detrital apatite fission-track signature of post-LGM sediments in the Ross Sea.....	412
Liberato G.P., Cornamusini G., Zurli L., Conti P., Calver C., Meffre S. & Talarico F.M. - Stratigraphic insights across Permian-Triassic boundary in southern Gondwana: comparison between Victoria Land (Antarctica) and Tasmania (Australia)	413
Liberato G.P., Cornamusini G., Zurli L., Woo J., Corti V., Oh J.-R. & Talarico F.M. - Sandstones provenance study of the Permian-Triassic sequences at Allan Hills (Victoria Land, Antarctica): evidence from petrographic framework	414
Pelorosso B., Bonadiman C., Ntafflos T., Gregoire M., Zanetti A. & Coltorti M. - Ultramafic cumulates from Harrow Peaks, (NVL, Antarctica): the first stages of the Ferrar magmatism.....	415

Rocchi S. & Smellie J.L. - Plutons, dykes and volcanoes as witnesses of lithospheric thinning, faulting and necking in northern Victoria Land, Antarctica	416
Rocchi S., D’Orazio M., Masotta M. & Folco L. - In memory of Pietro Armienti	417
Tolotti R., Caffau M., Colizza E. & Sauli C. - Holocene Antarctic Ice Sheet evolution in the Ross Sea: new evidences from the North-Western Basin	418
Tribuzio R., HenjesKunst F., Gerdes A. & Braga R. - Geochemical, isotopic and geochronological constraints on formation of boninite-type rocks at the Paleopacific margin of Gondwana.....	419
Vignaroli G., Rossetti F., Di Vincenzo G., Balsamo F., Gerdes A., Theye T. & Ghezzi C. - Late Cambrian-Early Ordovician orogenic construction along the paleo-Pacific margin of Gondwana, USARP Mountains, Northern Victoria Land (Antarctica)	420
Zurli L., Cornamusini G., Liberato G.P., Talarico F.M., Woo J., Conti P. & Corti V. - Stratigraphic comparison between Victoria Land (Antarctica) and Tasmania (Australia) Late-Palaeozoic glaciogenic sequences.....	421
Zurli L., Cornamusini G., Liberato G.P., Talarico F.M., Woo J. & Corti V. - Provenance study of Late Palaeozoic Ice Age sequences in Victoria Land (Antarctica): petrography and geochronology.....	422
Zurli L., Perotti M., Talarico F.M., Cornamusini G., McKay R.M., De Santis L., Kulhanek D.K. & the IODP Expedition Scientists - Petrographic characterization of gravel size clasts of the IODP_exp374 cores: implication for Miocene ice flows in the Ross Sea region (Antarctica)	423
S18. Mechanical, chemical and hydraulic interactions in seismogenic fault zones	424
Aben F.M. - Rupture-induced off-fault damage: Laboratory quantification and implications for fault mechanics	425
Cerchiari A., Remitti F., Mittempergher S., Festa A., Lugli F. & Cipriani A. - Interrelated changes in fluid sources and stress field orientation during the seismic cycle reconstructed for an exhumed analogue of the subduction megathrust shallow portion.....	426
Collettini C., Tesei T., Scuderi M.M., Carpenter B.M. & Viti C. - Beyond Byerlee Friction, Weak Faults and Implications for Slip Behaviour	427
Coppola M., Billi A., Stagno V., Cavallo A., Correale A., Fondriest M., Nazzari M., Paonita A., Romano C., Viti C. & Vona A. - Fluid-mediated deformation processes along the seismogenic Mt. Morrone fault zone (Central Apennines, Italy).....	428
Corsi G., Balsamo F., Bezerra F.H.R. & Salvioli-Mariani E. - Structural inheritance, fluid flow and intraplate seismicity along the Samambaia Fault, NE Brazil	429
Fondriest M., Mecklenburgh J., Passelegue F.X., Artioli G., Nestola F., Spagnuolo E. & Di Toro G. - Pseudotachylytes alteration and their loss from the geological record	430
La Rosa A., Pagli C., Molli G., Casu F., De Luca C., Pieroni A. & D’amato Avanzi G. - Growth of a sinkhole in a seismic zone of the northern Apennines (Italy).....	431
Malatesta C., Crispini L., Läufer A., Ildefonse B., Federico L. & Scarsi M. - Microstructural investigation of a prehnite-epidote bearing detachment horizon in granite (northern Victoria Land, Antarctica): influence of hydrothermal fluids on the fault mechanics.....	432
Marchesini B., Garofalo P.S., Menegon L., Mattila J. & Viola G. - Fluid-mediated, brittle-ductile cyclicity at seismogenic depth: Fluid record and deformation history of a fault system of the Svecofennian basement in SW Finland.....	433
Meneghini F., Aretusini S., Spagnuolo E., Harbord C. & Di Toro G. - Weakening mechanisms and rupture propagation along the Hikurangi margin frontal thrust: preliminary results from high speed friction experiments under controlled fluid pressure.....	434
Merico A., Giuliani L., Iezzi G., Pace B., Ferranti L., Cremona M., Scafa M., Nazzari M., Colella A. & Scarlato P. - Texture of tectonised calcite clasts from the San Benedetto-Gioia dei Marsi fault (central Italy).....	435
Mittempergher S., Bistacchi A., Di Toro G., Nielsen S. & Gukov K. - Roughness, off-fault damage and frictional melt distribution in an exhumed seismogenic fault: quantitative high resolution data from a Digital Outcrop Model study.....	436

Pizzati M., Balsamo B. & Storti F. - Influence of accommodated displacement upon microstructural and petrophysical properties of deformation bands and gouges affecting faulted high-porosity siliciclastic sediments (Rocca di Neto fault zone, Crotona Basin, Italy)	437
Raggiunti M., Keir D. & Pagli C. - Seismicity induced by fluid migration in the Main Ethiopian Rift	438
Vadacca L., Rossi D., Scotti A. & Buttinelli M. - Understanding the hydro-mechanical interaction in active fault zones by induced seismicity studies.....	439
S19. The interplay between magmatic systems and tectonics: insights from multidisciplinary approaches.....	440
Acquafredda P., Festa V., Fornelli A., Micheletti F. & Tursi F. - Controlled behavior of anatectic melts in the deep crust by regional tectonics and metamorphic conditions	441
Casini L., Maino M. & Montserrat L. - Frictional-viscous heating in strong elliptical inclusions during simple shear.....	442
Corvo' S., Langone A., Maino M., Cuccuru S., Oggiano G. & Seno S. - Petrological and geochronological constraints of a shallow intrusion into the Variscan medium-grade metamorphic sequence of the Asinara Island (Sardinia).....	443
Cuccuru S., Conte A.M., Naitza S., Oggiano G., Secchi F. & Puccini A. - Application of <i>in-situ</i> gamma-ray spectrometry to mapping intrusive complexes: examples from Sàrrabus igneous massif (SE Sardinia, Italy).....	444
Fazio E., Fiannacca P., Lombardo R., Tomaselli L., Vilardo F. & Cirrincione R. - A combined petro-structural study assisted by UAV-survey of mafic microgranular enclaves hosted by syn-tectonic tonalites at Rovaglioso outcrop (Calabria-Peloritani Orogen)	445
Fazio E., Fiannacca P., Lombardo R. & Cirrincione R. - Interaction between deformation and crustal melt generation at the plastic-brittle transition: a perspective from exhumed pseudotachylyte-bearing mylonites	446
Fazio E., Fiannacca P., Cirrincione R. & Mantani M.A. - A combined petrofabric and AMS approach to reveal the magmatism-tectonics link in a composite batholith: an example from the Serre Massif (Calabria, Italy).....	447
Fiannacca P., Fazio E., Russo D., Cirrincione R. & Pezzino A. - Submagmatic to solid-state shear-related deformation in late Variscan granitoids from a poly-orogenic mountain belt (Peloritani Mountains, southern Italy).....	448
Filippi M., Pulcini G., Rebay G., Zanoni D., Vergani D. & Spalla M.I. - Structure and petrography of mafic dykes from Val Camonica, Orobic Alps, Italy	449
Franceschini Z., Cioni R., Corti G., Sani F., Scaillet S., Isola I., Mazzarini F., Erbello A., Muluneh A., Keir D. & Brune S. - Recent volcano-tectonic evolution of the Ririba rift (southern termination of the Main Ethiopian Rift, East Africa).....	450
Gaggero L., Maino M., Cuccuru S. & Oggiano G. - Bimodal felsic-mafic volcano-plutonic magmatism associated to intramontane basins: the late-Variscan geodynamics recorded in North Sardinia (Italy)..	451
Liotta D., Brogi A. & Dini A. - Pliocene-Quaternary granitoids in the transfer zone of the Larderello geothermal area (Italy).....	452
Lombardo R., Fiannacca P., Basei A.S. & Cirrincione R. - Origin and evolution of post-collisional mafic granitoids (Capo Vaticano Promontory, Southern Calabria): geochemical and geochronological constraints.....	453
Olvera Garcia E., Bastesen E., Bianco C., Brogi A., Caggianelli A., Garduño Monroy V.H., Liotta D., Torabi A., Wheeler W.H. & Zucchi M. - Faults controlling ore deposits distribution in the Las Minas area (Mexico)	454
Roda M. & Zanoni D. - Multidisciplinary approach to test the thermal state of Biella pluton country rocks ...	455
Spieß R., Caggianelli A., Langone A., Stuart F., Bianco C., Zucchi M., Brogi A. & Liotta D. - The cooling, deformation and exhumation history of the late Miocene syn-tectonic Porto Azzurro pluton in a transfer zone (Elba Island, Italy)	456

Visalli R., Fazio E., Ortolano G., Alsop G.I., Pagano M. & Cirrincione R. - Semi-automated fabric analysis of strong rheologically contrasting mylonitic rocks: The example from the strike-slip Palmi shear zone.....	457
Zucchi M., Brogi A., Liotta D., Ruggieri G., Fregola R.A., Matera P.F., Dini A., Morelli G., Ventruti G. & Rimondi V. - Geothermal fluids flow and storage in faulted and folded metasiliciclastics (eastern Elba Island, Italy)	458
S20. Orogenesis and orogenic wedges: a multiscale and multitechnique approach	459
Argnani A., Manzi V., Lugli S. & Roveri M. - The Calabrian Arc orogenic wedge: a Messinian reconstruction	460
Barbero E., Delavari M., Dolati A., Pandolfi L., Marroni M., Saccani E. & Catanzariti R. - The Ganj Ophiolitic Complex reinterpreted as a Late Cretaceous volcanic arc: implications for the geodynamic evolution of the North Makran domain (SE Iran)	461
Barbero E., Delavari M., Dolati A., Pandolfi L., Marroni M., Saccani E., Chiari M., Luciani V. & Catanzariti R. - Preliminary stratigraphic and petrological data on the Durkan Complex (Makran accretionary wedge, SE Iran)	462
Basso J., Artoni A., Torelli L., Polonia A., Carlini M., Gasperini L. & Mussoni P. - The Plio-Pleistocene Bradano basin and the Southern Apennine Orogenic Wedge: evidences of accretion collision and segmentation of Apulian continental plate	463
Berardo G., Bonaccorso L., De Filippis G., Di Carlo L., Di Renzo M. E., Emili E., Gencarelli G., Iammarino C., Lavaroni F., Locchi M.E., Modesti M., Mosconi F., Pardo S., Perrotta V., Pignalberi F., Rinaldi F., Ruggiero G., Solfanelli M., Tedesco C., Valente M., Scuderi M., Curzi M., Marmoni G.M., Mercuri M. & Collettini C. - The M. Tancia regional thrust: geometric, kinematic and mechanical characterization within the Structural Geology course at La Sapienza.....	464
Berio L., Balsamo F., Bistacchi A., Mittempergher S. & Storti F. - Structural and paleofluid evolution during and after the growth of the Parmelan Anticline, Bornes Massif, Western Alps	465
Bitonte R., Bellentani G., Dall'igna M., Livio F., Ciabbarri F. & Scaramuzzo E. - Validation of structural and depositional models for a reservoir study in southern Apennines: uncertainty quantification by means of discrete geological scenarios.....	466
Cerchiari A. & Fagereng A. - Low temperature cyclical switching between brittle and ductile deformation inferred from microstructural analysis of quartz shear veins	467
Curzi M., Carminati E., Aldega L., Berra F., Billi A., Van der Lelij R. & Viola G. - Architecture and evolution of an extensionally-inverted thrust (Monte Tancia thrust, central Apennines, Italy): geological, structural, geochemical, and K-Ar geochronological constraints.....	468
D'Intino N., Scisciani V. & Esestima P. - The superposition of non-coaxial extensional events in rift basins: a case study from the Utsira High	469
Federico L., Maino M., Crispini L. & Capponi G. - Paleo-depth of fault activity: testing a method based on inversion of fault-slip data.....	470
Lacombe O. - Thick-skinned tectonics in orogenic forelands: the external western Alps and the western US Laramide Province case studies.....	471
Lucca A., Storti F., Balsamo F., Clemenzi L., Fondriest M., Burgess R. & Di Toro G. - Out-of-sequence thrusting from marine to phreatic conditions in the Gran Sasso Massif, Central Apennines, Italy	472
Panini F., Bettelli G., Carlini M., Fioroni C., Nirta G. & Remitti F. - A new geological map of the high Sillaro Valley (Northern Apennines, Italy)	473
Rossi F.P., Corrado S., Lugli S., Manzi V., Reghizzi M., Roveri M. & Schito A. - Multiproxy Burial and Exhumation Numerical Modelling of the late Miocene succession of the Eastern Romagna Apennines: implications for Messinian salinity crisis-related deposits diagenetic products	474
Sabbatino M., Vitale S., Consorti L., Corradetti A., Arienzo I., Cipriani A. & Parente M. - Multidisciplinary study of the Miocene forebulge unconformity in central-southern Apennines	475
Sternai P. - Present-day uplift of the European Alps: mechanisms and relative contributions.....	476

Succo A., Mittempergher S., Lucca A., Bistacchi A., Meda M. & Storti F. - From layer-parallel shortening and duplexing to fold tightening and strike-slip compartmentalization in the External Dinarides orogenic wedge: the case of platform carbonates folded in the Pag anticline.....	477
Tavani S., Corradetti A., Sabbatino M. & Mazzoli S. - Geological record of the transition from induced to self-sustained subduction in the Oman Mountains.....	478
Velicogna M., Princivalle F., Petrelli M., Venier M. & Lenaz D. - U-Pb detrital zircon geochronology of Cretaceous-Eocene flysch basins of the N-E Adria plate	479
S21. Active tectonics and seismotectonics between Northern Apennines and Southern Alps as a complex thrust belt - foredeep system	480
Bonadeo L., Frigerio C., Ferrario M.F., Livio F., Michetti A.M., Bitonte R., Scaramuzzo E., Zerboni A., Porat N., Fioraso G., Irace A., Catanzariti R., Da Prato S., Ellero A. & Ottria G. - A multidisciplinary approach to the structural setting and morphotectonics of the Eastern Monferrato Arc: new constraints to the seismic hazard assessment of a slowly deforming area	481
Bragato P.L. - Tectonic cycles over a human lifetime: multi-decadal periodicity of strong seismicity in Italy (Alps-Apennines system)	482
Busetti M., Zgur F., Dal Cin M., Vrabec M., Baradello L., Böhm G., Brancatelli G., Caffau M., Furlani S., Picotti S. & Zampa L.S. - The effects of the Cenozoic Dinaric and Alpine orogenies in the Gulf of Trieste (North Adriatic Sea).....	483
Cheloni D., Giuliani R., D'Agostino N., Mattone M., Bonano M., Fornaro G., Lanari R., Reale D. & Atzori S. - Active seismotectonics of the Northern Apennines: insights from the 2012 Emilia earthquake sequence.....	484
Dal Cin M., Busetti M., Böhm G., Picotti S., Zgur F. & Camerlenghi A. - 3D velocity depth model and seismic imaging of geological structures in the Gulf of Trieste (North Adriatic Sea), at the south-western edge of Dinarides and Alps	485
Galderisi A., Galli P. & Trotta O. - Evidence of surface ruptures along the Norcia fault during the Mt. Vettore fault earthquake. Passive activation induced by Coulomb stress change?	486
Mascandola C., Massa M., Barani S., Albarello D., Lovati S., Martelli L., Poggi V. & Morasca P. - Seismo-stratigraphic model of the Po Plain (Italy).....	487
Mele M., Zuffetti C., Aliverti Piuri E., Bersezio R., Giudici M., Comunian A. & Contini D. - Geophysical imaging of a buried faulted anticline: the San Colombano hill, southern Po Plain of Lombardy (Northern Italy).....	488
Nirta G., Piccardi L., Bonini M., Corti G., Montanari D., Moratti G. & Sani F. - Active normal faulting in the Garfagnana and Lunigiana basins. New geomorphic and geological constraints	489
Patricelli G. & Poli M.E. - Seismotectonic characterization of active faults in the LGM plain between Udine and Pozzuolo (Friuli, NE Italy)	490
Romano M.A., Peruzza L., Garbin M., Priolo E. & Picotti V. - The Montello thrust image obtained with a dense, high-quality seismic network (Southeastern Alps, Italy)	491
Sbarra P., Burrato P., Tosi P., Vannoli P., De Rubeis V. & Valensise G. - A new approach to estimate the depth of historical earthquakes: seismotectonic implications for the Northern Apennines and the southern Po Plain.....	492
Scaramuzzo E., Livio F., Di Capua A. & Bitonte R. - Crustal wedge structure in the Mt. Campo dei Fiori Area (Lugano - Lake Maggiore area): foredeep implication.....	493
Serpelloni E., Anderlini L., Pintori F., Vannucci G., Tolomei C., De Martini P.M. & Pezzo G. - Kinematics and seismic potential of the Eastern Southern Alps from space geodetic data.....	495
Teloni S., Invernizzi C., Costa M. & Pierantoni P.P. - Seismogenic structures in the onshore-offshore Padano-Adriatic foothills between Emilia Romagna and Marche: a tentative modelling for the evaluation of risks in seismically quiet areas	496
Tirincanti E., Roccheggiani M. & Menichetti M. - Geometry and kinematics of the Umbro-Marchean Apennines in the Adriatic foreland.....	497

Zampieri D., Burrato P. & Vannoli P. - The Schio-Vicenza fault system: field and seismological evidences and open questions.....	498
Zanchi A., Deaddis M., De Amicis M., Marchetti M., Ravazzi C. & Vezzoli G. - The Holocene deformed succession of Montodine (Cremona, Italy): evidence of recent tectonic activity?.....	499
Zuffetti C. & Bersezio R. - Late Quaternary sedimentation and tectonics in the Po Basin: field evidences at the Po Plain-Apennines border (Lombardy).....	500
S22. From seismic source to fault using multidisciplinary approaches: the central and southern Apennines as natural laboratory	501
Barreca G., Scarfi L., Gross F., Monaco C. & De Guidi G. - Fault pattern and seismotectonic potential at the south-western edge of the Ionian Subduction system (southern Italy): new field and geophysical constraints.....	502
Brozzetti F., Mondini A.C., Pauselli C., Mancinelli P., Cirillo D., Guzzetti F. & Lavecchia G. - Mainshock anticipated by intra-sequence ground deformations: insights from multiscale field and SAR interferometric measurements.....	503
Buttinelli M., Petracchini L., Maesano F.E., Scrocca D., D'Ambrogi C., Di Bucci D., Marino M., Capotorti F., Cavinato G., Bigi S. & RETRACE-D working group,, - The impact of high structural complexity on seismotectonics: hints and lessons learned in the areas of the 2016-2018 central Italy seismic sequence in the framework of the RETRACE-3D project.....	504
Caporali A., Zurutuza J. & Bertocco M. - A time dependent model of elastic stress in the Central Apennines, Italy.....	505
Cirillo D., Brozzetti F., de Nardis R., Lavecchia G., Orecchio B., Presti D. & Totaro C. - Multidisciplinary approach for 3D fault geometry reconstruction: an example from Calabrian-Lucanian boundary in the Mt. Pollino area (Southern Apennines-Italy).....	506
Cortinovis S., Balsamo F., Fondriest M., La Valle F. & Di Toro G. - Structural architecture and microstructural properties of the seismogenic Monte Marine fault zone, central Apennines (Italy).....	507
De Guidi G., Barreca G., Bella D., Brighenti F., Carnemolla F., Figlioli A., Menichetti M., Roccheggiani M. & Monaco C. - Multidisciplinary survey methods of the Fiandaca-Pennisi fault zone reactivated during the 26th December 2018 coseismic and postseismic event.....	508
de Nardis R., Pandolfi C., Monachesi G., Cattaneo M., Marzorati S., Cirillo D., Ferrarini F., Brozzetti F. & Lavecchia G. - High-sampling of multi-layered crust-scale seismogenic deformation in Central-Eastern Italy.....	509
Ferranti L., Pepe F., Barreca G., Meccariello M. & Monaco C. - Multi-temporal tectonic evolution of Capo I Granitola and Sciacca foreland transcurrent faults (Sicily channel).....	510
Forlano S., Ferranti L. & Milano G. - Recent and active tectonics in the Campanian Plain based on integration of fault kinematics and seismological data: preliminary results.....	511
Lavecchia G., de Nardis R., Pandolfi C., Monachesi G., Cattaneo M., Marzorati S., Cirillo D., Ferrarini F. & Brozzetti F. - Three-dimensional pattern of lithospheric compression in central Italy – Geodynamic implication.....	512
Maraio S., Villani F., Serri L., Sapia V., Improta L. & Bruno P.P. - Ultra-shallow imaging of a surface rupture fault of the 30 October 2016 Mw 6.5 central Italy earthquake from multidisciplinary geophysical approach.....	513
Menichetti M., Tirincanti E. & Roccheggiani M. - Earthquake ruptures geometries as tools for seismic hazard assessment.....	514
Montone P. & Mariucci M.T. - The shallow crust in Central Italy depicted by geophysical deep well logs.....	515
Nappi R., Paoletti V., Gaudiosi G., Luiso P., Cella F., Florio G. & Fedi M. - A multi-method approach to characterize the geometry of the Paganica and Matese seismogenic faults (Central-Southern Apennines, Italy).	516
Porreca M., Fabbrizzi A., Azzaro S., Pucci S., Del Rio L., Pierantoni P.P., Giorgetti C., Roberts G. & Barchi M.R. - 3D reconstruction of the M. Vettore seismogenic fault system (Central Apennines, Italy): cross-cutting relationship with the M. Sibillini Thrust.....	517

Puliti I., Pizzi A., Benedetti L., Di Domenica A. & Fleury J. - Evolution of an active fault system in an extensional context: the case of the Mt. Vettore system in the central Apennines and insights in its segmentation pattern.....	518
Scarpa R. - The southern Italy 1980 earthquake and the rupture processes of large earthquakes in Italy.....	519
Trippetta F., Barchi M.R., Borromeo O., Mastellone D., Rosset G. & De Paola N. - Seismic velocity variations of carbonates across the Apennines	520
Villani F., Maraio S., Bruno P.P., Improta L., Wood K., Civico R., Baccheschi P., Sapia V., Pucci S., Brunori C.A., De Martini P.M., Pantosti P.M., Conti P. & Doglioni C. - High-resolution seismic profiling in the Castelluccio basin: new constraints on the shallow subsurface of the 30 October 2016 Mw 6.5 Norcia earthquake fault (central Italy).....	521
Zambrano M., Corradetti A., Tavani S., Pitts A., Seers T.D. & Tondi E. - Roughness evaluation of the Monte Vettoreto active fault after the massive 2016 seismic sequence of Central Apennines, Italy	522
S23. Analogue and numerical modelling of geological processes: linking observation, interpretation and prediction	523
Cocco F. & Funedda A. - An attempt at modelling the lithosphere of Sardinia block and surroundings: relationships among isostatic disequilibrium, geomorphic features and neotectonics.....	524
Corbi F. - Improving subduction megathrusts seismic hazard assessment: a proof of concept based on analog modelling and machine learning.....	525
Corti G., Nencini R. & Skyttå P. - Modelling the influence of pre-existing brittle fabrics on the development and architecture pull-apart basins	526
Lanzi C., Trasatti E. & Battaglia M. - Unveiling the engine of mid-term deformations at Ischia resurgent caldera (Italy) using remote sensing and in situ data.....	527
Maestrelli D., Bonini M., Corti G., Montanari D. & Moratti G. - Collapsed calderas vs inherited fabrics: insights from analogue modelling	528
Maestrelli D., Bonini M., Corti G., Montanari D. & Moratti G. - Interplay between rift propagation and inherited crustal fabrics: a case study from the Trans-Mexican Volcanic Belt (Mexico).....	529
Massaro L., Adam J. & Jonade E. - New Granular Rock-Analogue Materials (GRAM) for simulation of multi-scale fault and fracture processes.....	530
Regorda A., Lardeaux J.-M., Roda M., Marotta A.M. & Spalla M.I. - How many subductions in the Variscan orogeny? Insights from numerical models	531
Ruch J. - Combining analogue experiments with ground deformation from space to study volcano tectonic processes.....	532
Spreafico M.C., Sternai P. & Agliardi F. - Rock-slope failure after deglaciation: rapid response or progressive long-term evolution? Insights from numerical modelling	533
Zwaan F., Corti G., Keir D. & Sani F. - Factors controlling the structural architecture of continental rift margins: insights from analogue centrifuge models.....	534
S24. Geology-hydrogeology of karst environments and modeling of preferential flow in variably saturated fractures.....	535
Arcari A., Dall'Aglio M., Balsamo F., Menezes D., Bagni F. & Bezerra F.H.R. - Structural control on karst system in folded layered carbonates, Potiguar basin, NE Brazil.....	536
Berardi M., Vurro M. & Portoghese I. - Modeling hydraulic conductivities of an infiltration trench.....	537
Bordoni M., Valentino R., Meisina C. & Bittelli M. - Detailed analysis of soil-atmosphere interactions in two sample sites in Oltrepò Pavese	538
Caputo M.C., Nimmo J.R. & Perkins K.S. - Characterization of Episodic Recharge in a Fractured and Karst Coastal Aquifer by Episodic Master Recession Analysis.....	539
Caputo M.C., De Carlo L., Masciale R., Perkins K.S. & Turturro A.C. - Combined approaches to provide evidence of preferential flow in a layered vadose zone during artificial rainfall	540

Gentile P., Iaia C., Liso I.S. & Parise M. - Occurrence of flash floods in the karst environment of Apulia (Southern Italy).....	541
Liso I.S. & Parise M. - Micro-climatic aspects at the karst system of Vora Bosco (Salento, Southern Italy)....	542
Liso I.S., Masciopinto C. & Parise M. - Hydrogeological model to study natural water flow in karstified and fractured aquifers.....	543
Martinelli G. & Tamburello G. - Influence of tectonic CO ₂ degassing on the occurrence of earthquake precursors.....	544
Nimmo J.R. & Perkins K.S. - Preferential flow dynamics in unsaturated zone hydrology.....	545
Perkins K.S. & Nimmo J.R. - Estimation of Preferential Flow Contributions to Aquifer Recharge Based on Hydrograph Analysis.....	546
Piccini L. & Poggetti E. - Hydrodynamic of karst springs in metamorphic carbonate rocks: the case of Apuan Alps (Tuscany, Italy).....	547
Pintori F., Serpelloni E., Longuevergne L., Belardinelli M.E., Gualandi A. & Scoccimarro E. - Water storage changes and crustal deformation in karst regions: examples from the Venetian Southern Alps.....	548
Turturro A.C., Nimmo J.R., Perkins K.S. & Caputo M.C. - Evidence of No Preferential Flow in Porous Rock by Testing the Validity of the Darcy-Buckingham Law in a Centrifugal Field.....	549
Vigna B. & Fiorucci A. - Conceptual models related to underground circulation in carbonate aquifers ¹	550
Wang X. & Jourde H. - Numerical models of karst processes.....	551
Zucchini A., Cirilli S., Comodi P., Mitillo N., Lanzafame G. & Frondini F. - The influence of the dolomitization process on texture and porosity of carbonates.....	552
S25. Geosciences for disaster risk reduction: problems, solutions and perspective.....	553
Allasia P., Godone D., Wrzesniak A., Notti D., Baldo M., Faccini F., Elter F.M. & Poggi F. - The importance of integrated monitoring approach: the case study of Arzeno (Graveglia Valley - Ligurian Apennine, Italy).....	554
Alvioli M., Guzzetti F. & Marchesini I. - Automatic delineation of slope units and terrain classification of Italy.....	555
Brunetti M.T., Peruccacci S., Rossi M., Marchesini I., Denti B., Solimano M., Martinotti M.E., Balducci V. & Guzzetti F. - Regional landslide early warning systems in Italy.....	556
Buondonno E., Cubellis E., Delizia I., Luongo G. & Ricci F. - Ischia Island: a model for sustainable development and natural risk mitigation.....	557
Cappello A., Ganci G., Bilotta G., Corradino C., Hérault A. & Del Negro C. - Assessing lava flow risk at Etna volcano.....	558
Chiappetta G.D., Gervasi A., Festa R.L. & La Rocca M. - Seismic site effects in the area of Tortora (Northern Calabria).....	559
Fiorucci F., Ardizzone F., Santangelo M., Bucci F., Allasia P., Alvioli M., Baldo M., Bianchi C., Brunetti M.T., Cavalli M., Clerissi F., Crema S., Donnini M., Giordan D., Guzzetti F., Marchesini I., Marchi L., Melillo M., Mondini A.C., Peruccacci S., Reichenbach P., Rossi M., Salvati P. & Cardinali M. - The 2016 Central Italy Seismic Sequence: emergency and post-emergency activities.....	560
Gioia E. & Marincioni F. - Analyzing flood risk perception to connect forecasting and alert agencies with the community: the case of the life primes project.....	561
Gioia E. & Marincioni F. - A comparison between empirical landslide predictive models applied to the Marche region (Central Italy).....	562
Giuffrè M., Benigni M.S., Coltella M., Martelli L., Pietrosante A. & Romani M. - Seismic microzonation and analysis of the Emergency Limit Condition - Useful tools for the seismic risk mitigation.....	563
Grezio A., Ardizzone F., Bucci F., Guzzetti F. & Marzocchi W. - Seismic- and Meteo-induced Landslides in Emilia Romagna.....	564
Marchesini I., Salvati P., Rossi M., Donnini M., Guzzetti F., Sterlacchini S., Zazzeri M., Cappellini G. & Voltolina D. - A statistical procedure used for the flood hazard zonation at national scale.....	565

Martinotti M.E., Marchesini I., Rossi M., Peruccacci S. & Guzzetti F. - Local indexes, based on a nationwide threshold, for rainfall-induced landslides	566
Marzocchi W., Falcone G. & Taroni M. - Progresses and challenges for Operational Earthquake Forecasting in Italy	567
Meletti C., Marzocchi W., D'Amico V., Luzi L., Martinelli F., Pace B., Rovida A., Visini F. & MPS Working Group - MPS19: the updated seismic hazard model of Italy as an example of state-of-the-art in PSHA	568
Pepe A., Zhao Q., Kubanek J., Falabella F., Yin J., Yu D., Lin N., Ma G. & Liu M. - Differential Synthetic Aperture Radar Experiments over the Ocean-Reclaimed Lands of Shanghai: Long-term flood Hazard Modeling and Urban Infrastructure Monitoring	569
Peruccacci S., Brunetti M.T., Gariano S.L., Melillo M., Rossi M. & Guzzetti F. - National and regional empirical rainfall thresholds for possible shallow landslide occurrence in Italy	570
Porfido S., Nappi R., Gaudiosi G., Alessio G. & Michetti A.M. - Between ethics and territorial planning: the value of the ESI-2007 scale	571
Rossi M., Guzzetti F., Salvati P., Donnini M., Napolitano E. & Bianchi C. - Modelling societal landslide risk in Italy	572
Rossi M., Marchesini I., Martinotti M.E., Brunetti M.T., Peruccacci S., Balducci V. & Guzzetti F. - Landslide early warning: lessons learned after 10-year experience in Italy	573
Sterlacchini S., Zazzeri M., Cappellini G., Voltolina D., Marchesini I., Salvati P., Rossi M., Donnini M. & Guzzetti F. - A GIS-based application to support decision makers in preparedness and response to flood-related risks	574
Versace P., Capparelli G., Spolverino G. & Galasso L. - Laboratory tests on pyroclastic soil to simulate the infiltration processes responsible of landslide trigger	575
Versace P., Capparelli G., Biondi D., Cruscomagno F., Vacha D. & Galasso L. - People's vulnerability to floods: the EVIL model	576
S26. Approaches for evaluation and protection of groundwater resources.....	577
Apollaro C., Fuoco I., De Rosa R., Vespasiano G., Gabriele B., Mancuso R., Criscuoli A. & Figoli A. - Natural polluted waters in Calabria Region (Italy): preliminary data on arsenic contamination and treatment	578
Barbagli A., Guastaldi E., Giannuzzi M., Borsi I., Lotti F., Basile P., Schembri M. & Sapiano M. - 3-Dimensional geological reconstruction of the Maltese archipelago geology as a tool for a better understanding on the main Maltese groundwater bodies	579
Barbero D., Bucci A., De Luca D.A., Forno M.G. & Lasagna M. - A new thermal model of the shallow aquifer by statistical temperature distribution in the Piedmont Po Plain (NW Italy).....	580
Barbero D., Bucci A., De Luca D.A., Forno M.G. & Lasagna M. - Thermal data as a tool for groundwater flow velocity determination in aquifer recharge areas.....	581
Capizzi P., Martorana R., Favara R., Albano L., Bonfardeci A., Costa N. & Gagliano A.L. - Geophysical and hydrological model of "Barcellona-Milazzo plain" groundwater body	582
Chiaudani A., Di Curzio D. & Rusi S. - The role of snow melting and rainfall on the discharge and physico-chemical characteristics of springs: a statistical analysis in Central Apennines	583
Corniello A., Del Gaudio E., Ducci D. & Stellato L. - The well fields of the Maggiore e Tifata mountains (Campania Region): new hydrochemical and isotopic data	584
Deluca F., Mongelli G., Paternoster M., Sinisi R. & Zhu Y. - Rare earth element speciation in volcanic groundwater: the Mount Vulture aquifer (Southern Italy).....	585
Di Curzio D. & Rusi S. - Stationary and non-stationary geostatistics to model 3-D hydraulic conductivity distribution: a case study in the southern Po river plain.....	586
Ducci D. & Sellerino M. - A Modified AVI Model to Map Groundwater Vulnerability to Contamination: case studies in Southern Italy	587

Iván V., Masetti M., Mádl-Szőnyi J., Pollicino L.C. & Stevenazzi S. - Spatial and statistical analysis of factors influencing groundwater vulnerability on the study area of the Gömör-Torna Karst (Hungary and Slovakia)	588
Petrella E., Chiari A., Segadelli S. & Celico F. - Hydrogeological and isotopic characterization of an ophiolite aquifer (Monte Zirone, Northern Apennines, Italy)	589
Portoghese I., Demichele F., Fidelibus D. & Vurro M. - Infiltration ponds adopted for treated wastewater disposal: a risk-assessment approach in the Apulia region.....	590
Raimondo M., Chelli A., Celico F., Iacumin P. & Petrella E. - Hydrogeological and isotopic investigation to define the hydrological behaviour of a complex landslide: a case study in the Northern Apennines (Italy)	591
Severini E., Pinardi M., Racchetti E., Celico F. & Bartoli M. - Evidences of diffuse water and nitrate input via river-groundwater interactions in a regulated river: flood irrigation as main driver?	592
Stellato L., Allocca V., Arienzo M., Coda S., De Vita P., Di Rienzo B., D'Onofrio A., Ferrara L., Marzaioli F. & Trifuoggi M. - Multi-disciplinary study to characterize groundwater flow processes and quality in an agriculture impacted volcanic-sedimentary coastal aquifer in the archaeological site of Cumae (Phlegraean Fields, southern Italy).....	593
Vespasiano G., Apollaro C., Muto F., Tripodi V., Fuoco I., Dotsika E. & De Rosa R. - Hydrogeochemical, isotopic and geological characterization of the thermal areas in the Calabria region	594
S27. Geologic and geothematic mapping in a dynamic country: maps, database and data dissemination	595
Bahrambeygi B., Moeinzadeh H. & Alavipanh SK. - Effect of types of Atmospheric corrections on Hyperspectral processing in lithology mapping, Case study of Iranian S-E Ophiolitic lithology	596
Berti D., Basi M., Bonomo R., Marino M., Pampaloni M.L., Ricci V., Rossi M., Silvestri S. & Urbani A. - Geological mapping and first level seismic microzonation in Abruzzo: case studies in the Aventino basin (southern Abruzzo).....	597
Carta R., Muraro C., Bonomo R., D'Angelo S., Martarelli L., Papasodaro F., Ricci V. & Vita L. - The Lithological Database of the CARG Project	598
Conti P., Cornamusini G. & Carmignani L. - Geological map of the Italian Northern Apennines (Emilia-Romagna, Marche, Tuscany, Umbria regions) at 1:250.000 scale, with GIS vector data	599
d'Atri A., Barale L., Borghi A., Dino G., Favero-Longo S.E., Gambino F., Giardino M., Lombardo V., Martire L., Perotti L. & Piana F. - The Piemonte Ornamental Stones geodatabase compliant with the "GeoPiemonte Map" web-GIS service.....	600
Federico L., Scarsi M., Crispini L., Piazza M. & Capponi G. - Mapping a HP belt and its sedimentary cover: interplay between tectonics and sedimentation (Ligurian Alps, Italy)	601
Funari V., Rizzieri A. & Dinelli E. - SuoliBo-HD: preliminary results of the high-density magnetic mapping of the Bologna topsoils from the public green and other outcropping urban soils.....	602
Montepeloso M., Zanchetta S., Berio L. & Zanchi A. - Geological-Structural map of the Late Carboniferous – Early Permian Orobic basin in the upper Brembana Valley (Orobic Alps, N Italy).....	603
Taussi M., Borghi W., Gliaschera M., Del Moro S., Di Gregorio A. & Renzulli A. - Defining the potential of Ground Source Heat Exchanger (GSHE) through a geological-based thermal modelling: a GIS approach applied to Fano Municipality (Marche region, Italy).....	604
Vennari C., Casarano D., Marchesini I., Salvati P., Parise M. & Lollino P. - A regional geodatabase on landslide, flood and sinkholes for civil protection application.....	605
S28. Geomorphological Hazards and Cartography	606
Bonomo A.E., Prosser G., Rizzo G., Bentivenga M. & Acito A.M. - The negative space: a geological journey into an open pit quarry.....	607
Bordoni M., Lucchelli L., Corradini B. & Meisina C. - Reconstruction of lithotechnical terrain units for the assessment of shallow landslides hazard in Oltrepò Pavese (northern Italy).....	608

Bosino A., Bernini A., Botha G., Omran A., Pellegrini L. & Maerker M. - Using web-based applications to enhance traditional geomorphic mapping: a case study of the Upper Mkhomazi River basin, KwaZulu-Natal, South Africa.....	609
Cafiso F., Cappadonia C., Rotigliano E. & Sulli A. - Seismic-induced rockfalls: Correlations between the slope aspect and seismic source.....	610
Conoscenti C., Martinello C., Agnesi V. & Rotigliano E. - Gully erosion susceptibility maps in Sicily through data mining techniques	611
Gemignani C.A., Giacomelli S., Leonelli G. & Chelli A. - Historical maps as source of information on temporal distribution of landslide events in the Northern Apennines	612
Giacomelli S., Lammoglia T. & Sgavetti M. - A SRTM-based geomorphometric analysis aimed at (neo) tectonics activity detection: a case study from an intracratonic area (Mato Grosso, Brazil)	613
Giacomelli S., Sgavetti M., Bertoni D., Rossi V., Lammoglia T., Leonelli G. & Chelli A. - Integrated use of geomorphological and open-access remote sensing data: examples from different case studies.....	615
Guarino P.M., Amanti M., Chiessi V., Fiano V., Guarneri E.M., Marasciulo T., Olivetta L., Pistocchi L., Roma M., Serafini R. & Vitale V. - Landslides in the Sibillini Mountains National Park (Central Apennines, Italy)	616
Guerra C., Guerra V. & Nesci O. - Geomorphological cartography in urban coastal settlements: the Rimini town case history (Emilia-Romagna, Italy).....	617
Ivy-Ochs S., Martin S., Viganò A., Campedel P., Rossato S., Vockenhuber C. & Rigo M. - Historic and pre-historic landslide activity along the lake Garda - Brenta Group channel area (NE Italy)	618
Leonelli G., Celico F., Petrella E., Francese R. & Chelli A. - Integrating GIS and tree-ring techniques for characterizing surface movements of landslides in the Northern Apennines: challenges, strengths and limitations at the Carobbio study site	619
Martinello C., Rotigliano E., Conoscenti C. & Agnesi V. - Investigation of prediction errors in the landslide susceptibility statistical models through multiple nested MARS analyzes: application in the Caldera area of Ilopango (El Salvador, C.A.)	620
Nsengiyumva J.B., Valentino R., Sobio Y., Mizero J., Nsengiyumva F., Bordoni M. & Meisina C. - Site-specific to large-scale landslides susceptibility assessment in Rwanda	621
Rossi M., Santangelo M., Alvioli M., Marchesini I., Cardinali M., Bucci F. & Fiorucci F. - Composite landslide susceptibility maps.....	622
Rotigliano E., Martinello C., Cappadonia C. & Agnesi V. - Integrating pixel analysis into slope units landslide susceptibility mapping: an application to the Imera river basin	623
Valletta A., Cavalca E., Savi R. & Segalini A. - Advantages of innovative automatic inclinometers applied to landslides monitoring for early warning activities	624
S29. Recent advances in fluid geochemistry in active volcanic and geothermal areas: following Mariano Valenza	625
Aiuppa A. - Global trends in volcanic gas composition	626
Bini G., Chiodini G., Cardellini C., Vougioukalakis G.E. & Bachmann O. - Estimating the energetic budget of hydrothermal systems using diffuse emission of CO ₂ : the case of Nisyros (Greece).....	627
Brugnone F., Calabrese S., D'Alessandro W., Li Vigni L. & Parello F. - The impact of Mt. Etna's ash plume on the chemical composition of meteoric deposition	628
Cabassi J., Capecciacci F., Magi F., Vaselli O., Tassi F., Montalvo F., Esquivel I., Grassa F. & Caprai A. - Water and dissolved gas geochemistry at Coatepeque, Ilopango and Chanmico volcanic lakes (El Salvador, Central America)	629
Calabrese S., Li Vigni L., Brugnone F. & Capasso G. - The precious "scientific heritage" of Mariano Valenza: the unknown history of Ludovico Sicardi and the birth of the modern volcanology	630
Cardellini C., Chiodini G., Frondini F., Caliro S., Avino R., Bagnato E., Beddini G. & Rosiello A. - Carbon dioxide diffuse emission in volcanic and hydrothermal areas: monitoring volcanic activity and impact on carbon global emissions.....	631

Chiodini G. & Caliro S. - Magma degassing episodes at volcanoes in hydrothermal activity.....	632
Chiodini G., Beddini G., Caliro S., Cardellini C., Frondini F. & Rosiello A. - Measuring and interpreting CO ₂ and advective heat fluxes at regional scale: the case of Apennines, Italy.....	633
Di Martino R.M.R., Camarda M. & Gurrieri S. - The monitoring of hydrogen and carbon dioxide at Stromboli volcano.....	634
Di Martino R.M.R., Capasso G. & Camarda M. - The on-field measurements of ¹³ C/ ¹² C of the CO ₂ improve the consolidated practices of volcano monitoring.....	635
Falcone E.E., Federico C., Boudoire G., Brusca L., Bellomo S. & Saiano F. - Geochemistry of trace metals and REE in low temperature hydrothermal areas in Vulcano Island (Aeolian Islands, Italy).....	636
Fazi S., Tassi F., Rossetti S., Pratesi P., Ceccotti M., Cabassi J., Capechciacci F., Venturi S. & Vaselli O. - The microbial community structure in a meromictic volcanic lake (Lake Averno, Italy).....	637
Federico C., Bellomo S., Brusca L., Calabrese S., D'Alessandro W., Falcone E.E. & Longo M. - Bioavailability of trace and ultratrace elements in soils in the Mt. Etna volcanic area: the role of the emission source and insights on their mobility in the interstitial solution.....	638
Fuoco I., Apollaro C., Vespasiano G., Timpano A., Cundari F. & De Rosa R. - Chemical weathering rates and CO ₂ consumption in the eastern sector of Sila Massif (Calabria, Italy) inferred from riverine water chemistry.....	639
Gagliano A.L., Daskalopoulou K. & D'Alessandro W. - New perspectives in geothermal CH ₄ output estimation.....	640
Grezio A., Costa A., Rouwet D. & Chiodini G. - Modelling the dynamics of volcanic lakes: Nyos Lake (Cameroon) and Albano Lake (Italy).....	641
Lelli M., Taramaeli M., Ariph K., Sadock J., Pisani P., Pasqua C., Principe C., Mnzava F., Armadillo E., Rizzello D. & Mkangala A. - Relationships between CO ₂ soil degassing and regional/local fault systems in the Kiejo-Mbaka geothermal prospect (Tanzania).....	642
Li Vigni L., D'Alessandro W., Cardellini C., Daskalopoulou K., Calabrese S. & Brugnone F. - Preliminary study on geogenic degassing through the big karstic aquifers of Greece.....	643
Mancini A., Frondini F., Capezuoli E., Galvez Mejia E., Lezzi G., Matarazzi D., Brogi A. & Swennen R. - Travertine masses from western Central Italy and natural Earth degassing: an approach to evaluate the geogenic CO ₂ flux.....	644
Meloni F., Vaselli O., Nisi B., Rappuoli D., Cabassi J. & Bianchi F. - Geochemical features of the shallow aquifer in the former mining area of Abbadia San Salvatore (Tuscany, central Italy).....	645
Moretti R., Moune S.--, Robert V., Bonifacie M., Jessop D.-- & Komorowski JC. - A geochemical reappraisal of the hydrothermal system of La Soufrière of Guadeloupe (French West Indies) with implications for unrest.....	646
Nicodemi L., Brogi A., Capezuoli E., D'Orazio M., Fulignati P. & Zanchetta G. - Unravelling hypogean mineralizing fluids from the geochemistry of epigeal travertines: insights from central-southern Tuscan (Italy).....	647
Procesi M., Cinti D., Cabassi J., Capechciacci F., Caracausi A., Pizzino L., Fazi S. & Casentini B. - Does the anthropogenic lake Ex-Snia, in the centre of Rome, simulate the characteristics of a volcanic lake?.....	648
Randazzo P., Caracausi A., Apollaro C., Cardellini C., Chiodini G., Paternoster M., Rosiello A. & Aiuppa A. - Fluid geochemistry and CO ₂ output in the southern Apennine (Italy): Preliminary results.....	649
Rosiello A., Cardellini C., Chiodini G., Frondini F. & Caliro S. - CO ₂ Earth Degassing in Southern Italy: quantification and source identification of the main regional aquifers of the Southern Apennines and Gargano Promontory.....	650
Rouwet D., Tamburello G., Procesi M., Venturi S., Santi A., Chiodini G., Pecoraino G., Ricci T., Cabassi J. & Tassi F. - Resuming volcanic surveillance at Lake Albano: updates on the dissolved gas content and vertical temperature profiles.....	651
Ruggieri G., Orlando A. & Borrini D. - The synthesis of fluid inclusions: from the lab to geothermal wells...	652
Tamburello G. & Carbonara N. - Distribution of the thermal springs in the world in relation to active volcanic and tectonic areas.....	653

Tassi F. - Past and present of geochemical investigations on meromictic volcanic lakes: hints for the next future.....	654
Tassi F., Inostroza M., Sepúlveda J., Capecchiacci F. & Aguilera F. - Preliminary geochemical investigation of the Colpitas hydrothermal system, northern Chile.....	655
Tassi F., Cabassi J., Andrade C., Callieri C., Silva C., Viveiros F., Corno G., Vaselli O., Selmo E., Gallorini A., Ricci A., Giannini L. & Cruz J.V. - Mechanisms regulating CO ₂ and CH ₄ dynamics in the Azorean volcanic lakes (São Miguel Island, Portugal)	656
Venturi S., Cabassi J., Butturini A., Vazquez E., Pacini N., Tassi F., Vaselli O., Amalfitano S., Crognale S., Rossetti S., Harper D.M., Capecchiacci F. & Fazi S. - Tropical saline-alkaline lakes as a major source of greenhouse gases: evidence from lake Sonachi, Kenya	657
S30. Legacy and new applications of stable-isotope geochemistry.....	658
Boito M., Iacumin P. & Ogrinc N. - The link between groundwater and milk in the Parmigiano-Reggiano cheese production area: validation with the isotopic analysis for food traceability.....	659
Cavazzini G. - Inter-measurement determination of the isotopic composition of Sr (II).....	660
Dordoni M., Pennisi M., Agostini S., Dini A., Di Giuseppe P., Rielli A., Provenzale A., Bianchini G., Natali C., Marchina C. & Cidu R. - First isotopic analyses in fluid samples using MC-ICP-MS (NEPTUNE PLUS™): results on Boron-poor fluvial and rain water (Adige basin)	661
Doveri M., Stenni B., Gianecchini R., Petrini R., Ghezzi L., Dreossi G. & Menichini M. - Characteristics of hydrogen and oxygen stable isotopes in water from an area impacted by past-mining activity in southern Apuan Alps (Italy).....	662
Ghezzi L., Petrini R., Castorina F., Scotti C., Ottria G. & Bartelletti A. - Trace element composition and Sr-isotope ratio in wine, must and soil from a high-altitude vineyard in the Apuan Alps UNESCO Global Geopark (Italy).....	663
Lutman A., Petrini R. & Ghezzi L. - Chromium-isotope systematics, new insights from a contaminated area in the Friuli Venezia-Giulia Region.....	664
Maccelli C., Avanzinelli R., Casalini M., Nisi B., Vaselli O. & Mason P. - Heavy metals in surface waters and suspended solids from the Usciana River (Tuscany, central Italy).....	665
Macri A. & Iacumin P. - Paleoclimate reconstruction using freshwater organisms from prehistoric shell midden	666
Pennisi M., Agostini S., Dini A., Dordoni M., Di Giuseppe P., Rielli A., Provenzale A. & Rodushkin I. - Boron isotopic analyses in fluid samples - PTIMS <i>VERSUS</i> MC-ICP-MS (Neptune PLUS™).....	667
Regattieri E., Zanchetta G., Drysdale R.N., Giaccio B., Isola I., Mannella G., Nomade S. & Hellstrom J.C. - Hydrological significance of δ ¹⁸ O composition of speleothems and lakes carbonates from Apennine sites (Italy): a coherent hydrological framework for the Last Interglacial period.....	668
Rodushkin I., Pallavicin N. & Engström E. - Novel application of MC-ICP-MS for stable isotope measurements	669
Varrica D., Tamburo E., Alaimo M.G., Losno R. & Monna F. - Use of lead isotopic fingerprint in human scalp hair to identify potential sources of pollution in industrial Sicilian sites (Italy).....	670
Vaselli O., Tarchiani U., Nisi B. & Cabassi J. - Geochemical and isotopic investigation on underground waters affected by high sulfate contents.....	671
S31. Geochemistry of mercury: from noble metal to global pollutant.....	672
Acquavita A., Brandolin D., Felluga A., Maddaleni P., Meloni C., Poli L., Skert N. & Zanello A. - Mercury distribution and speciation in soils contaminated by historically mining activity: The Isonzo River plain (NE Italy).....	673
Bianchi F., Rappuoli D., Vaselli O., Nisi B. & Esposito A. - Distribution of mercury, antimony and arsenic in the terrains from the former mining area of Abbadia San Salvatore (Siena, central Italy).....	674

Cabassi J., Rimondi V., Yeqing Z., Vacca A., Vaselli O., Buccianti A. & Costagliola P. - 100 years of high GEM concentration in the Central Italian Herbarium and Tropical Herbarium Studies Centre (Florence, Italy)	675
Cabassi J., Di Bennardo F., Venturi S., Tassi F., Nisi B., Magi F., Ricci A., Picchi G. & Vaselli O. - Gaseous Elemental Mercury (GEM) fluxes from the soil of the hydrothermal area of Monterotondo Marittimo (Grosseto, Central Italy)	676
Covelli S., Langone L., Petranich E., Acquavita A., Giordano P. & Giani M. - Spatial and temporal distribution of mercury in the recent sediments of the Adriatic Sea	677
Fantozzi L., Marziali L., Valsecchi L., Schiavon A., Orrù A. & Guerrieri N. - First investigation of atmospheric mercury pollution around the chlor-alkali plant of Pieve Vergonte (Italian central Alps) ..	678
Magi F., Cabassi J., Capecciacci F., Giannini L., Nisi B., Pandeli E., Rappuoli D., Tassi F., Venturi S. & Vaselli O. - Mercury in groundwater from the Mt. Amiata area (central Italy).....	679
Monaci F., McLagan D.S., Rappuoli D., Huang H., Lei Y. D., Mitchell C.P.J. & Wania F. - Long-term monitoring and modeling of gaseous mercury concentrations around the abandoned mine of Abbadia San Salvatore: the potential of passive sampling for detecting variation patterns and effects of emission-reduction associated with remediation works	680
Pasquetti F., Zanchetta G., Vaselli O., Nisi B., Bianchi S., Mirri S. & Nannucci S.M. - New insight into Hg origin in the Orbetello lagoon (Tuscany, Italy).....	681
Petranich E., Pavoni E., Signore S. & Covelli S. - Mercury mobility in harbour sediments: evidence from selective sequential extraction and short-term microcosm resuspension experiments (northern Adriatic Sea, Italy).....	682
Pirrone N. - What are the major challenges that should be taken on board in supporting nations in the implementation of the Minamata convention on mercury.....	683
Valerio M., Ghezzi L. & Petrini R. - Mercury contamination in soils of an urban setting and the pathways of dispersion.....	684
Vaselli O., Nisi B., Rappuoli D., Cabassi J., Esposito A. & Tassi F. - Discontinuous monitoring of Gaseous Elemental Mercury in the former mining area of Abbadia San Salvatore (Siena, central Italy).....	685
S32. New developments and challenges in volcanology: insights from experimental, analytical and field studies	686
Cubellis E., Pappalardo L. & Petrosino P. - Eruptive dynamics during violent strombolian Vesuvius 1906 eruption.....	687
Del Bello E., Taddeucci J. & Scarlato P. - Investigating the behaviour of volcanic ash using controlled laboratory experiments	688
Di Salvo S., Avanzinelli R., Isaia R., Druitt T.H. & Francalanci L. - The role of new magma recharges and crystal-mush interaction in the Campanian Ignimbrite activity, revealed by geochemical and isotope micro-analyses	689
Frontoni A., Costa A., Vona A., Pistone M. & Romano C. - Rheology of particle-bearing suspensions: preliminary results	690
Frontoni A., Vona A., Giordano G., Viccaro M. & Romano C. - Clastogenic lava flow: the case study from Mount Etna	691
Ganci G., Cappello A., Bilotta G., Corradino C., Héroult A. & Del Negro C. - Monitoring of lava flow hazards: The December 24, 2018 Mt. Etna eruption.....	692
Giuliani L., Iezzi G., Casarin A., Piattelli V., Lanzafame G., Nazzari M., Ferlito C., Mollo S., Scarlato P., Trabucco F. & Colò M. - Textural variations along a vertical section of a distal portion of an Etnean lava flow	693
González-García D., Petrelli M., Behrens H., Vetere F., Morgavi D., Giordano D. & Perugini D. - Diffusive fractionation of trace elements between mixing melts: the experimental approach.....	694
Kazarian A., Cáceres F., Scheu B., Vona A., Misiti V., Dingwell D.B. & Romano C. - An experimental overview on the role of decompression on bubble formation in trachytic magma	695

Monaco L., Giaccio B., Palladino D.M., Gaeta M., Sottili G., Marra F., Castorina F., Nomade S., Pereira A. & Albert P.G. - Early explosive activity at Vico volcano, central Italy: a new perspective from proximal and distal sedimentary archives	696
Morgavi D., Spina L., Cannata A., Musu A., Campeggi C. & Perugini D. - AEOLUS: a laboratory to study bubble-bearing flow dynamics and geophysical signals through analogue volcanic eruption.....	697
Musu A., Morgavi D., Spina L., Corsaro R.A. & Perugini D. - Lava fountaining activity: the Collapsing Foam Layer Model applied to the 2000 – 2013 South-East Crater eruptive period (Mt. Etna, Italy).....	698
Petrelli M. & Zellmer G. - Volcanic plumbing system dynamics: unravelling rates and timescales of magma transfer, storage, and eruption	699
Pisello A., Vetere F.P., Murri M., Alvaro M., Rossi S., Holtz F. & Perugini D. - Viscosity of ultramafic melts during cooling: insights for emplacement of Martian lava flows.....	700
Primerano P., Giordano G., Vona A., De Vita S. & Morgavi D. - Rheological behavior of lava flows from Ischia Island (Campania, Italy).....	701
Rooyackers S., Morgavi D., Perugini D., Petrelli M., Vetere F., Stix J., Berlo K., Barker S. & Charlier B. - Basalt-rhyolite interaction timescales in the caldera-forming Halarauður eruption (Krafla, Iceland) constrained by chaotic mixing experiments	702
Rossi S., Petrelli M., Morgavi D., Vetere F.P., Almeev R.R., Astbury R.L. & Perugini D. - Role of magma mixing in the pre-eruptive dynamics of the Aeolian Islands volcanoes (Southern Tyrrhenian Sea, Italy).....	703
Sacco G., Caltabiano T., Salerno G. & Viccaro M. - SO ₂ flux and eruptive activity at Mt. Etna between the 2015 and 2016	704
Scarani A., Silleni A., Vona A., Romano C. & Giordano G. - Infrared thermography of pyroclast cooling across the glass transition temperature: effect of clast composition, porosity and dimension.....	705
Silleni A., Ryan A.G., Russell J.K., Vona A., Giordano G., Ort M. & Romano C. - The effects of interclast viscosity contrast in the welding ability of pyroclastic deposits	706
Spina L., Morgavi D., Cannata A. & Perugini D. - Experimental investigations on degassing behavior and related seismo-acoustic markers: the effect of complex conduit geometries	707
S33. Geosciences at school 2019	708
Antiga R., Cabella R., Elter F.M. & Massa A. - Design and experimentation of educational activities on Water resources in the underground: development of an experimental protocol to analyze the dynamics of infiltration, accumulation and exploitation processes in incoherent deposits.....	709
Antiga R., Cabella R., Coniglio L., Carpanese M.G., Elter F.M., Lodi C., Massa A., Parola C., Tarella G. & Tsakarisianos M.D. - To know the hydrogeological instability - study methods and its awareness: the case of Val Graveglia - Genova - Eastern Liguria	710
Artoni C., Bollati I.M. & Pelfini M. - Virtual geomorpholabs: simple games for geomorphorisk education....	711
Beccaceci A., Stacchiotti L. & Paris E. - Sustainable city: work together for a more sustainable life style	712
Belluzzo A., Bronzo L., Citron S., Di Stefano G., Favaroni A., Gazzola R., Gazzurra G., Giacomini P., Martella A., Merella M., Nicodemi L., Porta L., Bianucci G., Bosio G., Collareta A., Gioncada A., Landini W., Mollì G., Sarti G. & Borghini A. - ICA-LAB: un laboratorio di ricerca interdisciplinare nel Lagerstätte del deserto costiero di Ica (Perù)	713
Bonaccorsi E., Borghini A., Gioncada A. & Pieraccioni F. - The good, the bad and the ugly: a movie around the geoscience textbooks	714
Boniello A. & Paris E. - The virtual trip of Darwin, the geologist	715
Borghini A., Pieraccioni F., Gioncada A. & Bonaccorsi E. - What are the students' mental models of the Earth's inner structure?.....	716
Caironi V., Regazzola V., Lorenzetti S.C., Berra G., Coltro G. & Fumagalli P. - Project "What a show! Create a geological corner in your high school"	717
Ferretti M., Invernizzi C., Mazzoli S. & Carroll M.R. - Exploring the moon, using Earth's rocks and fossils: an earth science module.....	718

Garzarella A., Valentini A., Pace B., Liguori A., Michelangeli M.A. & Middle School Class B - From Physics to Geology: exploring the time and space”, an outreach and successful project to understand the Earth system and the earthquakes, through the use of the <i>Quakecaster</i> , awarded by Gran Sasso National Laboratory (LNGS), INFN (National Institute for Nuclear Physics), contest “Anch’io Scienziato 2019”	719
Lozar F. & Tonon M.D. - Climate education in the deep time perspective: working with teachers and students	720
Moroni B. - “HAVE YOU GOT A GREEN THUMB?” Hands-on experiences of kids’ and teens’ earth science education by inquiry-based methods	721
Occhioni M. - Earth Science in Opensim-based virtual worlds.....	722
Occhipinti S. - A PBL approach to enhance the sensitivity of students towards natural risks and hazards, in Italian schools	723
Occhipinti S. - a EGU-IGEO European chapter to promote the teaching learning of Earth science in all schools	724
Pauselli C., Musu A., Mancinelli P., Ercoli M., Porreca M., Azzaro S., Carboni F., Samperi L., Giorgetti C., Mirabella F., Barchi M., Minelli G., Moriconi A. & Martorana S. - Il terremoto: impariamo a conoscerlo. The earthquake: let’s get to know it	725
Pelfini M., Apuani T., Artoni C., Conforto A. & Bollati I. - How to exploit geodiversity in geoscience education activities?	726
Pelorosso B., Brombin V., Bertagnon A., Calore E., Forastieri F., Polastri L., Rolando V. & Vinciguerra E. - Alps in a box.....	727
Piangiamore G.L., Trolese P., Frione A. & Cortopassi P. - Social Emotional Learning (SEL) and earthquake: teaching through emotions meets Geoscience.....	728
Placuzzi E., Barbieri G., Berti M., Gasparotto G., Giura E., Rossi V., Squarzoni G., Vaiani S.C. & gli studenti del Liceo E. Ferrari, Cesenatico - Il Piano Lauree Scientifiche come strumento di didattica inclusiva: il contributo delle geoscienze.....	729
Punturo R., Fazio E., Fiannacca P., Ortolano G. & Cirrincione R. - The Floristella-Grottacalda Mineral Park (Sicily): a geological trip that becomes history, literature and memory of a territory.....	730
Realdon G. & Gravina T. - New opportunities for teacher professional development in Earth sciences: EGU Geoscience Fieldwork Officers Project	731
Scacchetti M. & Chicchi S. - Esperienze didattiche attorno a Valentina, balena fossile di 3.5 milioni di anni .	732
Scapellato B. - La circolazione oceanica	733
Scopesi C., Belmonte D., Briguglio A., Cabella R., Carbone C., Forchielli A. & Doria G. - Geosciences and museum: new frontiers in didactic for high school students	734
Seno S. & Lupi C. - Geoscience laboratory for primary school: an attempt for engaging young people in Earth Sciences.....	735
Stacchiotti L., Beccaceci A. & Paris E. - The scientific method between geology and history.....	736
Tonon M.D. & Caretto A. - The aesthetic approach to teaching geosciences and sustainable education	737
Zaccara Bertolini P., Foglia C., Classe IVF, Groppi E., Classe IIIH, Mantovani L., Tribaudino M., Artesi T. & Solzi M. - Pollution from magnetic minerals in leaves: an “Alternanza Scuola Lavoro” project in secondary schools in Parma and Torino	738

Probing the sorption capacity of Y Zeolite towards pharmaceutical compounds: a neutron powder diffraction study

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Due to their widespread use and slow natural degradation, pharmaceutical products are among the most common ubiquitous contaminants of waters and wastewaters. At present, pharmaceuticals removing from water systems through adsorption on synthetic microporous zeolites is considered the best compromise in terms of cost-effectiveness and eco-sustainability (Martucci et al., 2015; Rodeghero et al., 2016). In this work, two samples of Y zeolite (*i.e.*, Si/Al ratio=30) loaded with two different pharmaceutical compounds (*ibuprofen*, C₁₃H₁₈O₂ and *atenolol*, C₁₄H₂₂N₂O₃) were studied through neutron powder diffraction to determine zeolite sorption capacity and highlight host-guest interactions. Drug-loaded zeolites were obtained exchanging the as-synthesized form with deuterated ibuprofen and atenolol in aqueous solution for 140 h at room temperature and then washing with D₂O. Diffraction data were collected at the D2B beamline (ILL; Grenoble) at 4 K. Rietveld refinements were performed using the GSAS software (Larson & von Dreele, 1994), whereas extra-framework sites were located by difference Fourier maps and then optimized using EXPO2014 (Altomare et al., 2013) software to obtain reasonable bond lengths and angles and calculate the H atoms position. Results obtained from the cell parameters analysis confirmed the presence of extraframework molecules within the zeolite pores, which were located within the *supercage* through the difference Fourier maps analysis. Contrariwise, no coadsorbed water molecules were detected. Refinement of extraframework occupancies revealed the presence of higher amount of ibuprofen (33.68%) than atenolol (11.55%) within the zeolite pores. According to bond distances analysis, both molecules directly interact with the zeolite framework, thus guaranteeing the molecule immobilization and preventing from uncontrolled release phenomena. The analysis of structural parameters allowed calculating both ellipticity and Crystallographic Free Area (CFA), which highlighted strong differences among the two drug-zeolite systems. Compared to the bare zeolite (unloaded-Y=46.26), CFA values after molecules adsorption increase: *ibu*-Y=56.58 and *atn*-Y=48.16. On the contrary, after loading no evident differences in channel shape and geometry were detected, thus confirming the high flexibility of zeolite framework. Based on the obtained results, the Y zeolite efficiency in ibuprofen and atenolol adsorption has been proved and its possible exploitation as sorbent materials in water remediation treatments can be assumed.

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