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Editore	Titolo dell'articolo	Titolo della rivista	Data di approvazione richiesta finanziamento	Corresponding Author
ACS	Surface and Bulk Distribution of Fluorides and Ti ³⁺ Species in TiO ₂ Nanosheets: Implications on Charge Carrier Dynamics and Photocatalysis	The Journal of Physical Chemistry C	13/01/2020	Mario Chiesa
ACS	On the Surface Acid–Base Properties of Amorphous and Crystalline Mg ₂ SiO ₄ as Probed by Adsorbed CO, CO ₂ , and CD ₃ CN	ACS Earth and Space Chemistry	10/02/2020	Matteo Signorile
ACS	Impurity Effects on Habit Change and Polymorphic Transitions in the System: Aragonite–Calcite–Vaterite	Crystal Growth & Design	09/03/2020	Dino Aquilano
ACS	Gaussian Basis Sets for Crystalline Solids: All-Purpose Basis Set Libraries vs System-Specific Optimizations	Journal of Chemical Theory and Computation	16/03/2020	Lorenzo Maschio
ACS	Triggering Neurotransmitters Secretion from Single Cells by X-ray Nanobeam Irradiation	Nano Letters	31/03/2020	Federico Picollo
ACS	Feasibility and the Mechanism of Desorption of Phenolic Compounds from Activated Carbons	Industrial & Engineering Chemistry Research	05/06/2020	Giancarlo Cravotto
ACS	Disclosing the Interaction between Carbon Monoxide and Alkylated Ti ³⁺ Species: a Direct Insight into Ziegler–Natta Catalysis	The Journal of Physical Chemistry Letters	25/06/2020	Alessandro Piovano
ACS	Exfoliation Energy of Layered Materials by DFT-D: Beware of Dispersion!	Journal of Chemical Theory and Computation	01/07/2020	Piero Ugliengo

ACS	Molecular Catalysts with Intramolecular Re–O Bond for Electrochemical Reduction of Carbon Dioxide	Inorganic Chemistry	29/07/2020	Carlo Nervi
ACS	Mechanochemistry Applied to the Synthesis of X-ray Contrast Agent	ACS Sustainable Chemistry & Engineering	03/08/2020	Giancarlo Cravotto
ACS	Structure and Reactivity of Oxygen-Bridged Diamino Dicationic Copper(II) Complexes in Cu-Ion-Exchanged Chabazite Catalyst for NH ₃ -Mediated Selective Catalytic Reduction	Journal of the American Chemical Society	24/08/2020	Gloria Berlier
ACS	Elevated CO ₂ Impact on Common Wheat (<i>Triticum aestivum</i> L.) Yield, Wholemeal Quality, and Sanitary Risk	Journal of Agricultural and Food Chemistry	31/08/2020	Massimo Blandino
ACS	Chemoselective Homologation–Deoxygenation Strategy Enabling the Direct Conversion of Carbonyls into (n+1)-Halomethyl-Alkanes	Organic Letters	01/09/2020	Vittorio Pace
ACS	Thermoelasticity of Flexible Organic Crystals from Quasi-harmonic Lattice Dynamics: The Case of Copper(II) Acetylacetonate	The Journal of Physical Chemistry Letters	18/09/2020	Alessandro Erba
ACS	Changes in Skin Flavanol Composition as a Response to Ozone-Induced Stress during Postharvest Dehydration of Red Wine Grapes with Different Phenolic Profiles	Journal of Agricultural and Food Chemistry	25/09/2020	Luca Rolle
ACS	Room temperature Solid-State Lithium-ion Battery using LiBH ₄ -MgO composite Electrolyte	ACS Applied Energy Materials	15/01/2021	Marcello Baricco
ACS	Charge Density Analysis of Actinide Compounds from the Quantum Theory of Atoms in Molecules and Crystals	The Journal of Physical Chemistry Letters	10/02/2021	Alessandro Erba
ACS	Mechanistic insights into the role of iron, copper and carbonaceous component on the oxidative potential of ultrafine particulate matter	Chemical Research in Toxicology	19/02/2021	Ivana Fenoglio

ACS	Thermosetting Polyurethane Resins as Low-Cost, Easily Scalable, and Effective Oxygen and Moisture Barriers for Perovskite Solar Cells	ACS Applied Materials & Interfaces	09/03/2021	Claudia Barolo
ACS	The Impact of P3HT Regioregularity and Molecular Weight on the Efficiency and Stability of Perovskite Solar Cells	ACS Sustainable Chemistry & Engineering	18/03/2021	Pierluigi Quagliotto
ACS	Targeting Acute Myelogenous Leukemia using potent human dihydroorotate dehydrogenase inhibitors based on the 2-hydroxypyrazolo[1,5-a]pyridine scaffold: SAR of the biphenyl moiety	Journal of Medicinal Chemistry	23/03/2021	Marco Lolli
ACS	Chromium Environment within Cr-doped Silico-Aluminophosphate Molecular Sieves from Spin Density Studies.	The Journal of Physical Chemistry C	26/03/2021	Mario Chiesa
ACS	Spin multiplicity and solid-state electrochemical behaviour in charge transfer co-crystals of DBTTF/F4TCNQ	The Journal of Physical Chemistry C	01/04/2021	Agnese Giacomino
ACS	Ab initio Modeling of Multi-Wall: a general algorithm first applied to carbon nanotubes	The Journal of Physical Chemistry A	15/04/2021	Silvia Casassa
ACS	Mapping of structural changes induced by X-ray nanopatterning via nano-XRD and corresponding electrical effects	Crystal Growth & Design	12/05/2021	Marco Truccato
ACS	Controlled Periodic Illumination Enhances Hydrogen Production by over 50% on Pt/TiO ₂	ACS Catalysis	18/05/2021	Francesco Pellegrino
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ACS	Gold(I)-Catalyzed Reactivity of Furan-ynes with N-Oxides: Synthesis of Substituted Dihydropyridinones and Pyranones	The Journal of Organic Chemistry	28/05/2021	Cristina Prandi

ACS	Impact of Microwaves on Organic Synthesis and Strategies toward Flow Processes and Scaling Up	The Journal of Organic Chemistry	14/06/2021	Giancarlo Cravotto
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ACS	The electronic properties of the Ti sites in Ziegler-Natta catalysts	ACS Catalysis	09/07/2021	Elena Groppo
ACS	Chromatographic Fingerprinting Enables Effective Discrimination and Identification of High-Quality Italian Extra-Virgin Olive Oils	Journal of Agricultural and Food Chemistry	16/07/2021	Chiara Cordero
ACS	Foreseen Effects of Climate-Impacted Scenarios on the Photochemical Fate of Selected Cyanotoxins in Surface Waters	Environmental Science & Technology	20/07/2021	Davide Vione
ACS	Spectroscopic fingerprints of MgCl ₂ /TiCl ₄ nanoclusters determined by machine learning and DFT	The Journal of Physical Chemistry C	01/09/2021	Maddalena D'Amore
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ACS	Electronic Excitations in Crystalline Solids through the Maximum Overlap Method	Journal of Chemical Theory and Computation	16/09/2021	Lorenzo Maschio
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ACS	Water interaction with Fe ₂ NiP schreibersite (110) surface: a quantum mechanical atomistic perspective	The Journal of Physical Chemistry C	10/01/2022	Piero Ugliengo

ACS	Long-Range Spatial Distribution of Single Aluminium Sites in Zeolites	The Journal of Physical Chemistry Letters	27/01/2022	Enrico Salvadori
ACS	Computer Generated Realistic Interstellar Icy Grain Models: Physico-chemical Properties and Interaction with NH ₃	ACS Earth and Space Chemistry	22/03/2022	Piero Ugliengo
ACS	Designing Soluble PROTACs: Strategies and Preliminary Guidelines	Journal of Medicinal Chemistry	13/04/2022	Giulia Caron
ACS	Titration of Cu(I) sites in Cu-ZSM-5 by volumetric CO adsorption	ACS Applied Materials & Interfaces	20/04/2022	Matteo Signorile
ACS	Theoretical distribution of the ammonia binding energy at interstellar icy grains: a new computational framework	ACS Earth and Space Chemistry	24/05/2022	Piero Ugliengo
ACS	Assessing the Influence of Zeolite Composition on Oxygen-Bridged Diamino Dicopper(II) Complexes in Cu-CHA DeNO _x Catalysts by Machine Learning-Assisted X-ray Absorption Spectroscopy	The Journal of Physical Chemistry Letters	23/06/2022	Elisa Borfecchia
ACS	The Structure of Monomeric HydroxoCuII Species in Cu-CHA. A Quantitative Assessment	Journal of the American Chemical Society	11/07/2022	Mario Chiesa
ACS	Effect of inoculation with Lactobacillus buchneri and Lactocaseibacillus paracasei on the maize silage volatilome: the advantages of advanced 2D-chromatographic fingerprinting approaches	Journal of Agricultural and Food Chemistry	03/08/2022	Chiara Cordero
ACS	Ion Conductivity in Magnesium Borohydride Ammonia Borane Solid-State Electrolyte	The Journal of Physical Chemistry C	29/08/2022	Lorenzo Maschio

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ACS	Refinement of computational access to molecular physicochemical properties: from Ro5 to bRo5	Journal of Medicinal Chemistry	30/08/2022	Matteo Rossi Sebastiano
ACS	Targeting Acute Myelogenous Leukemia Using Potent Human Dihydroorotate Dehydrogenase Inhibitors Based on the 2-Hydroxypyrazolo[1,5-a]pyridine Scaffold: SAR of the Aryloxyaryl Moiety	Journal of Medicinal Chemistry	22/09/2022	Marco Lolli
ACS	Evaluation of the environmental fate of a semivolatile transformation product of ibuprofen, based on a simple two-media fate model	Environmental Science & Technology	06/10/2022	Davide Vione
ACS	Photoinduced Chloroamination Cyclization Cascade with N-Chlorosuccinimide: from N-(Allenyl)sulfonylamides to 2-(1-Chlorovinyl)pyrrolidines	The Journal of Organic Chemistry	20/10/2022	Polysena Renzi
ACS	Electron Paramagnetic Resonance Single Metal Atoms on Oxide Surfaces. Assessing the Chemical Bond through 17O Electron Paramagnetic Resonance	Accounts of Chemical Research	11/11/2022	Mario Chiesa
ACS	Emergence of order in origins-of-life scenarios on minerals surfaces: polyglycine chains on silica	Langmuir	24/11/2022	Gloria Berlier
ACS	Polypeptide chain growth mechanisms and secondary structure formation in glycine gas-phase deposition on silica surfaces	The Journal of Physical Chemistry B	03-gen-2023	Gloria Berlier
ACS	From lab to technical CO ₂ hydrogenation catalysts: understanding PdZn decomposition	ACS Applied Materials & Interfaces	10-gen-2023	Silvia Bordiga
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ACS	Quinoid-thiophene based Covalent Organic Polymers for High Iodine Uptake: when rational chemical design counterbalances low surface area and pores volume	ACS Applied Materials & Interfaces	08-mar-2023	Matteo Bonomo
ACS	New class of tunable choline bromide-based hydrophobic deep eutectic solvents for the extraction of bioactive compounds of varying polarity from a plant matrix	ACS Sustainable Chemistry & Engineering	17-apr-2023	Cecilia Cagliero
ACS	Short-range Electronic Interactions between Vanadium and Molybdenum in Bimetallic SAPO-5 Catalysts Revealed by Hyperfine Spectroscopy	The Journal of Physical Chemistry C	22-mag-2023	Mario Chiesa
ACS	One-pot, Telescoped Alkenylation of Amides via Stable Tetrahedral Intermediates as Lithium Enolate Precursors	Organic Letters	22-mag-2023	Marco Blangetti
ACS	A Fresh Look at a Well-known Solid: Structure, Vibrational Spectra, and Formation Energy of $m\text{NaNH}_2$	The Journal of Physical Chemistry C	06-giu-2023	Lorenzo Maschio
ACS	Is the imposition of diamond morphology on mineral inclusions a syngenetic or post-genetic process with respect to diamond formation?	Crystal Growth & Design	09-giu-2023	Marco Bruno
ACS	Synergic effect of isolated Ce^{3+} and Pt^+ species in UiO-66(Ce) for heterogeneous catalysis	ACS Catalysis	19-giu-2023	Silvia Bordiga
ACS	The quest for oral PROTAC drugs: evaluating the weaknesses of the screening pipeline	ACS Medicinal Chemistry Letters	19-giu-2023	Giulia Caron
ACS	Chamelogk: a chromatographic chameleonicity quantifier to design orally bioavailable beyond-Rule-of-5 drugs	Journal of Medicinal Chemistry	10-lug-2023	Giulia Caron
ACS	Thermoplasmonic in situ fabrication of nanohybrid electrocatalysts over gas diffusion electrodes for enhanced H_2O_2 Electrosynthesis	ACS Catalysis	11-lug-2023	Alberto Naldoni

ACS	Interfacial States in Au/reduced-TiO ₂ Plasmonic Photocatalysts Quench Hot Carriers Photoactivity	The Journal of Physical Chemistry C	27-lug-2023	Alberto Naldoni
ACS	Assessing Low-Cost Computational Methods against Structural Properties and Size Effects of Pt nanoparticles	The Journal of Physical Chemistry C	28-ago-2023	Alberto Ricchebuono
ACS	Influence of agronomic practices on the antioxidant compounds of pigmented wheat (<i>Triticum aestivum</i> spp. <i>aestivum</i> L.) and tritordeum (<i>Tritordeum martinii</i> A. Pujadas, nothosp. nov.) genotypes	Journal of Agricultural and Food Chemistry	28-ago-2023	Massimo Blandino
ACS	Nanoporous Titanium Oxynitride Nanotube Metamaterials with Deep Subwavelength Heat Dissipation for Perfect Solar Absorption	ACS Photonics	31-ago-2023	Alberto Naldoni
ACS	The role of in situ/operando IR spectroscopy in unraveling adsorbate-induced structural changes in heterogeneous catalysis	Chemical Reviews	12-set-2023	Elena Groppo
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ACS	The effect of different evaporation rates on gypsum habit: mineralogical implications for natural gypsum deposits	Crystal Growth & Design	02-nov-2023	Andrea Cotellucci
ACS	Understanding Ionic Diffusion Mechanisms in Li ₂ S Coatings for Solid-state batteries: Development of a Tailored Reactive Force Field for Multiscale Simulations	The Journal of Physical Chemistry C	03-nov-2023	Maddalena D'Amore
ACS	Stability and Formation of the Li ₃ PS ₄ /Li, Li ₃ PS ₄ /Li ₂ S, and Li ₂ S/Li Interfaces: A Theoretical Study	Langmuir	22-nov-2023	Anna Maria Ferrari

ACS	Unravelling the molecular structure of zeolite-octyl methoxycinnamate hybrid UV filters: a combined spectroscopic and computational approach	The Journal of Physical Chemistry C	28-nov-2023	Lorenzo Mino
ACS	Copper-catalyzed continuous-flow transfer hydrogenation of nitroarenes to anilines: a scalable and reliable protocol	Organic Process Research & Development	30-nov-2023	Katia Martina
ACS	DegraderTCM: a computational-sparing approach for predicting Ternary Degradation Complexes	ACS Medicinal Chemistry Letters	01-dic-2023	Matteo Rossi Sebastiano
ACS	Seeking for Innovation with Magnetic Resonance Imaging Paramagnetic Contrast Agents: Relaxation Enhancement via Weak and Dynamic Electrostatic Interactions with Positively Charged Groups on Endogenous Macromolecules	Journal of the American Chemical Society	18-dic-2023	Eliana Gianolio