Maddalena D'Amore

List of Publications by Year
in descending order

30	725	516710 16	526287 27
papers	citations	h-index	g-index

32	32	32	717
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A periodic hybrid DFT approach (including dispersion) to MgCl2-supported Zieglerâ€“Natta catalysts â€“ 1: TiCl4 adsorption on MgCl2 crystal surfaces. Journal of Catalysis, 2012, 286, 103-110.	6.2	103
2	Surface Investigation and Morphological Analysis of Structurally Disordered MgCl₂and MgCl₂/TiCl₄Zieglerâ€“Natta Catalysts. ACS Catalysis, 2016, 6, 5786-5796.	11.2	83
3	Probing the Coordinative Unsaturation and Local Environment of Ti³⁺â€¦Sites in an Activated Highâ€Yield Zieglerâ€“Natta Catalyst. Angewandte Chemie - International Edition, 2015, 54, 4857-4860.	13.8	65
4	Revisiting the identity of Î´-MgCl2: Part I. Structural disorder studied by synchrotron X-ray total scattering. Journal of Catalysis, 2020, 385, 76-86.	6.2	51
5	Periodic Hybrid DFT Approach (Including Dispersion) to MgCl₂-Supported Zieglerâ€“Natta Catalysts. 2. Model Electron Donor Adsorption on MgCl₂ Crystal Surfaces. Journal of Physical Chemistry C, 2013, 117, 24345-24353.	3.1	47
6	Periodic and High-Temperature Disordered Conformations of Polytetrafluoroethylene Chains:Â An ab Initio Modeling. Journal of the American Chemical Society, 2006, 128, 1099-1108.	13.7	46
7	Spectroscopic Evidences for TiCl₄/Donor Complexes on the Surface of MgCl₂-Supported Zieglerâ€“Natta Catalysts. Journal of Physical Chemistry C, 2018, 122, 5615-5626.	3.1	33
8	Conformational Behavior and Magnetic Properties of a Nitroxide Amino Acid Derivative in Vacuo and in Aqueous Solution. Journal of Physical Chemistry A, 2003, 107, 6264-6269.	2.5	27
9	Electron Localization Function and Maximum Probability Domains analysis of semi-ionic oxides crystals, surfaces and surface defects. Computational and Theoretical Chemistry, 2015, 1053, 315-321.	2.5	25
10	Revisiting the identity of Î´-MgCl2: Part II. Morphology and exposed surfaces studied by vibrational spectroscopies and DFT calculation. Journal of Catalysis, 2020, 387, 1-11.	6.2	25
11	The Influence of Alcohols in Driving the Morphology of Magnesium Chloride Nanocrystals. ChemCatChem, 2017, 9, 1782-1787.	3.7	24
12	The Bond Analysis Techniques (ELF and Maximum Probability Domains) Application to a Family of Models Relevant to Bio-Inorganic Chemistry. Structure and Bonding, 2013, , 119-141.	1.0	19
13	Nitrogen substitutional defects in silicon. A quantum mechanical investigation of the structural, electronic and vibrational properties. Physical Chemistry Chemical Physics, 2019, 21, 20939-20950.	2.8	19
14	Binding of Nucleic Acid Components to the Serpentinite-Hosted Hydrothermal Mineral Brucite. Astrobiology, 2018, 18, 989-1007.	3.0	18
15	Disordered Chain Conformations of Poly(tetrafluoroethylene) in the High-Temperature Crystalline Form I. Macromolecules, 2004, 37, 9473-9480.	4.8	17
16	Characterization and Modeling of Reversible CO₂ Capture from Wet Streams by a MgO/Zeolite Y Nanocomposite. Journal of Physical Chemistry C, 2019, 123, 17214-17224.	3.1	17
17	A quantum mechanical study of TiCl3Î±, Î² and Î³ crystal phases: geometry, electronic structure and magnetism. Physical Chemistry Chemical Physics, 2009, 11, 11264.	2.8	15
18	Elucidating the Interaction of CO2 in the Giant Metalâ€“Organic Framework MIL-100 through Large-Scale Periodic Ab Initio Modeling. Journal of Physical Chemistry C, 2019, 123, 28677-28687.	3.1	15

#	Article	IF	Citations
19	Substitutional boron and nitrogen pairs in diamond. A quantum mechanical vibrational analysis. Carbon, 2019, 146, 709-716.	10.3	10
20	Spectroscopic Fingerprints of MgCl2/TiCl4 Nanoclusters Determined by Machine Learning and DFT. Journal of Physical Chemistry C, 2021, 125, 20048-20058.	3.1	9
21	Interface Between Alkylammonium Ions and Layered Aluminophosphates Materials: A Combined Theoretical and Experimental Study. Chemistry of Materials, 2008, 20, 4980-4985.	6.7	7
22	On the structure of superbasic (MgO)_n sites solvated in a faujasite zeolite. Physical Chemistry Chemical Physics, 2018, 20, 18503-18514.	2.8	7
23	Effects of molecular dynamics and solvation on the electronic structure of molecular probes. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	5
24	Inelastic Neutron Scattering Investigation of MgCl₂ Nanoparticle-Based Zieglerâ€“Natta Catalysts for Olefin Polymerization. ACS Applied Nano Materials, 2020, 3, 11118-11128.	5.0	5
25	Disordered Rock-Salt Type Li2TiS3 as Novel Cathode for LIBs: A Computational Point of View. Nanomaterials, 2022, 12, 1832.	4.1	5
26	Quasi-Hexagonal to Lepidocrocite-like Transition in TiO2 Ultrathin Films on Cu(001). Journal of Physical Chemistry C, 2021, 125, 10621-10630.	3.1	4
27	Effect of Internal Donors on Raman and IR Spectroscopic Fingerprints of MgCl2/TiCl4 Nanoclusters Determined by Machine Learning and DFT. Materials, 2022, 15, 909.	2.9	4
28	The NV0 defects in diamond: A quantum mechanical characterization through its vibrational and Electron Paramagnetic Resonance spectroscopies. Journal of Physics and Chemistry of Solids, 2022, 160, 110304.	4.0	3
29	The NVâ¯â‹¯N+ charged pair in diamond: a quantum-mechanical investigation. Physical Chemistry Chemical Physics, 2021, 23, 18724-18733.	2.8	2
30	Characterization of the negatively charged NV defect through the spin density distribution and the hyperfine coupling constants. Journal of Physics and Chemistry of Solids, 2021, , 110506.	4.0	0