

Maddalena D'Amore

List of Publications by Year in descending order

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Version: 2024-02-01

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papers

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citations

516681

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717
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#	ARTICLE	IF	CITATIONS
1	A periodic hybrid DFT approach (including dispersion) to MgCl ₂ -supported Ziegler-Natta catalysts 1: TiCl ₄ adsorption on MgCl ₂ crystal surfaces. <i>Journal of Catalysis</i> , 2012, 286, 103-110.	6.2	103
2	Surface Investigation and Morphological Analysis of Structurally Disordered MgCl ₂ and MgCl ₂ /TiCl ₄ Ziegler-Natta Catalysts. <i>ACS Catalysis</i> , 2016, 6, 5786-5796.	11.2	83
3	Probing the Coordinative Unsaturation and Local Environment of Ti ³⁺ Sites in an Activated High-Yield Ziegler-Natta Catalyst. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 4857-4860.	13.8	65
4	Revisiting the identity of $\hat{\Gamma}$ -MgCl ₂ : Part I. Structural disorder studied by synchrotron X-ray total scattering. <i>Journal of Catalysis</i> , 2020, 385, 76-86.	6.2	51
5	Periodic Hybrid DFT Approach (Including Dispersion) to MgCl ₂ -Supported Ziegler-Natta Catalysts. 2. Model Electron Donor Adsorption on MgCl ₂ Crystal Surfaces. <i>Journal of Physical Chemistry C</i> , 2013, 117, 24345-24353.	3.1	47
6	Periodic and High-Temperature Disordered Conformations of Polytetrafluoroethylene Chains: An ab Initio Modeling. <i>Journal of the American Chemical Society</i> , 2006, 128, 1099-1108.	13.7	46
7	Spectroscopic Evidences for TiCl ₄ /Donor Complexes on the Surface of MgCl ₂ -Supported Ziegler-Natta Catalysts. <i>Journal of Physical Chemistry C</i> , 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. <i>Journal of Physical Chemistry A</i> , 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. <i>Computational and Theoretical Chemistry</i> , 2015, 1053, 315-321.	2.5	25
10	Revisiting the identity of $\hat{\Gamma}$ -MgCl ₂ : Part II. Morphology and exposed surfaces studied by vibrational spectroscopies and DFT calculation. <i>Journal of Catalysis</i> , 2020, 387, 1-11.	6.2	25
11	The Influence of Alcohols in Driving the Morphology of Magnesium Chloride Nanocrystals. <i>ChemCatChem</i> , 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. <i>Structure and Bonding</i> , 2013, , 119-141.	1.0	19
13	Nitrogen substitutional defects in silicon. A quantum mechanical investigation of the structural, electronic and vibrational properties. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 20939-20950.	2.8	19
14	Binding of Nucleic Acid Components to the Serpentinite-Hosted Hydrothermal Mineral Brucite. <i>Astrobiology</i> , 2018, 18, 989-1007.	3.0	18
15	Disordered Chain Conformations of Poly(tetrafluoroethylene) in the High-Temperature Crystalline Form I. <i>Macromolecules</i> , 2004, 37, 9473-9480.	4.8	17
16	Characterization and Modeling of Reversible CO ₂ Capture from Wet Streams by a MgO/Zeolite Y Nanocomposite. <i>Journal of Physical Chemistry C</i> , 2019, 123, 17214-17224.	3.1	17
17	A quantum mechanical study of TiCl ₃ , $\hat{\Gamma}^2$ and $\hat{\Gamma}^3$ crystal phases: geometry, electronic structure and magnetism. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 11264.	2.8	15
18	Elucidating the Interaction of CO ₂ in the Giant Metal-Organic Framework MIL-100 through Large-Scale Periodic Ab Initio Modeling. <i>Journal of Physical Chemistry C</i> , 2019, 123, 28677-28687.	3.1	15

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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 MgCl ₂ /TiCl ₄ 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 MgCl ₂ Nanoparticle-Based Ziegler-Natta Catalysts for Olefin Polymerization. ACS Applied Nano Materials, 2020, 3, 11118-11128.	5.0	5
25	Disordered Rock-Salt Type Li ₂ TiS ₃ 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 TiO ₂ 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 MgCl ₂ /TiCl ₄ Nanoclusters Determined by Machine Learning and DFT. Materials, 2022, 15, 909.	2.9	4
28	The NV ⁰ 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 NV ⁻ 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