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List of Publications by Year
in descending order

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Version: 2024-02-01

36	703	471477	552766
papers	citations	17 h-index	26 g-index

36	36	36	1084
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	An atomistic characterization of the interplay between composition, structure and mechanical properties of amorphous geopolymer binders. Journal of Non-Crystalline Solids, 2016, 434, 53-61.	3.1	57
2	Size-dependent permittivity and intrinsic optical anisotropy of nanometric gold thin films: a density functional theory study. Optics Express, 2013, 21, 11827.	3.4	52
3	A molecular dynamics study of the role of molecular water on the structure and mechanics of amorphous geopolymer binders. Journal of Chemical Physics, 2016, 145, 134706.	3.0	49
4	Degradation Mechanism of Methyl Mercury Selenoamino Acid Complexes: A Computational Study. Inorganic Chemistry, 2011, 50, 2366-2372.	4.0	41
5	Environmental Mercury Chemistry â€“ In Silico. Accounts of Chemical Research, 2019, 52, 379-388.	15.6	40
6	Adsorption of Uranyl Species onto the Rutile (110) Surface: A Periodic DFT Study. Chemistry - A European Journal, 2012, 18, 1458-1466.	3.3	37
7	Computational study of the ground state properties of iodine and polyiodide ions. Theoretical Chemistry Accounts, 2009, 122, 119-125.	1.4	32
8	Computational studies on the interactions among redox couples, additives and TiO2: implications for dye-sensitized solar cells. Physical Chemistry Chemical Physics, 2010, 12, 14609.	2.8	32
9	Interactions of the N3 dye with the iodide redox shuttle: quantum chemical mechanistic studies of the dye regeneration in the dye-sensitized solar cell. Physical Chemistry Chemical Physics, 2011, 13, 15148.	2.8	28
10	Chalcogenophilicity of Mercury. Inorganic Chemistry, 2011, 50, 3791-3798.	4.0	26
11	Characterization of grapheneâ€“fullerene interactions: Insights from density functional theory. Chemical Physics Letters, 2013, 582, 115-118.	2.6	26
12	Computational Studies of the Interaction between Ruthenium Dyes and Xâ¯ and X2â¯, X = Br, I, At. Implications for Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2010, 114, 15165-15173.	3.1	25
13	Incorporation of water into olivine during nebular condensation: Insights from density functional theory and thermodynamics, and implications for phyllosilicate formation and terrestrial water inventory. Meteoritics and Planetary Science, 2015, 50, 578-589.	1.6	25
14	Computational Studies of Structural, Electronic, Spectroscopic, and Thermodynamic Properties of Methylmercury-Amino Acid Complexes and Their Se Analogues. Inorganic Chemistry, 2010, 49, 870-878.	4.0	24
15	Adsorption and Cluster Growth of Vanadium on TiO₂(110) Studied by Density Functional Theory. Journal of Physical Chemistry C, 2008, 112, 4622-4625.	3.1	23
16	Interface exchange coupling in Co nanoparticles dispersed in a Mn matrix. Journal of Physics Condensed Matter, 2010, 22, 436005.	1.8	20
17	Properties of polythiophene and related conjugated polymers: a density-functional study. Physical Chemistry Chemical Physics, 2005, 7, 2714.	2.8	18
18	Microstructural analysis of Warkâ€Lovering rims in the Allende and Axtell <scp>CV</scp>3 chondrites: Implications for highâ€temperature nebular processes. Meteoritics and Planetary Science, 2016, 51, 743-756.	1.6	17

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19	Relationship between dyeâ€“iodine binding and cell voltage in dyeâ€sensitized solar cells: A quantumâ€mechanical look. Journal of Computational Chemistry, 2012, 33, 2492-2497.	3.3	16
20	A First Principles Study on Charge Dependent Diffusion of Point Defects in Rutile TiO2. Journal of Physical Chemistry C, 2010, 114, 19649-19652.	3.1	15
21	A computational investigation of adsorption of organics on mineral surfaces: Implications for organics delivery in the early solar system. Earth and Planetary Science Letters, 2014, 408, 355-361.	4.4	15
22	Substitution Effects on the Water Oxidation of Ruthenium Catalysts: A Quantum-Chemical Look. Journal of Physical Chemistry C, 2015, 119, 242-250.	3.1	15
23	Adsorption of 3d Transition Elements on a TiO₂(110) Surface. Journal of Physical Chemistry C, 2008, 112, 19616-19619.	3.1	14
24	Computational studies of the interactions of Iâ^' and I3 â^' with TiO2 clusters: implications for dye-sensitized solar cells. Theoretical Chemistry Accounts, 2011, 129, 199-208.	1.4	14
25	Quantum-Chemical Study of the Diffusion of Hg(0, I, II) into the Ice(Ih). Journal of Physical Chemistry C, 2012, 116, 5151-5154.	3.1	10
26	Adsorption of Na and Hg on the Ice(Ih) Surface: A Density-Functional Study. Journal of Physical Chemistry C, 2010, 114, 2941-2946.	3.1	6
27	Hydrogen Isotope Fractionation in the Epidoteâ€“Hydrogen and Epidoteâ€“Water Systems: Theoretical Study and Implications. ACS Earth and Space Chemistry, 2018, 2, 1029-1034.	2.7	5
28	The hydration of periclase: Atomistic insights from quantum-chemical look. Chemical Physics, 2020, 532, 110694.	1.9	4
29	Theoretical Studies of Structural, Energetic, and Electronic Properties of Clusters. Zeitschrift Fur Physikalische Chemie, 2008, 222, 387-405.	2.8	3
30	Effect of Ligand Adsorption on the Electronic Properties of the PbS(100) Surface. Langmuir, 2020, 36, 13312-13319.	3.5	3
31	Density Functional Theory Driven Analysis of the Interplay among Structure, Composition, and Oxidation State of Titanium in Hibonite, Spinel, and Perovskite. ACS Earth and Space Chemistry, 2021, 5, 544-552.	2.7	3
32	Structural, energetic and vibrational properties of oxidized mercury in the gas and aqueous phases. Computational and Theoretical Chemistry, 2021, 1198, 113186.	2.5	3
33	Energetics of substituted polyhedral oligomeric silsesquioxanes: a DFT study. MRS Communications, 2015, 5, 519-524.	1.8	2
34	Hydrogen Isotope Fractionation in the Talcâ€“Serpentineâ€“Bruciteâ€“Water System: Theoretical Studies and Implications. ACS Earth and Space Chemistry, 2021, 5, 880-889.	2.7	2
35	A First-Principles Investigation of Lithium and Sodium Ion Diffusion in C₆₀ Molecular Solids. Journal of Physical Chemistry C, 2022, 126, 4259-4266.	3.1	1
36	The Role of Aluminum Substitution on the Stability of Substituted Polyhedral Oligomeric Silsesquioxanes. Zeitschrift Fur Physikalische Chemie, 2016, 230, 1005-1014.	2.8	0