Devis Di Tommaso

List of Publications by Year
in descending order

64	1,769	236925 25	302126 39
papers	citations	h-index	g-index

74	74	74	2208
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Bridging atomistic simulations and thermodynamic hydration models of aqueous electrolyte solutions. Journal of Chemical Physics, 2022, 156, 024502.	3.0	1
2	Porous nanographene formation on Î³-alumina nanoparticles via transition-metal-free methane activation. Chemical Science, 2022, 13, 3140-3146.	7.4	8
3	A Database of Solution Additives Promoting Mg²⁺ Dehydration and the Onset of MgCO₃ Nucleation. Crystal Growth and Design, 2022, 22, 3080-3089.	3.0	5
4	Resolving nanoscopic structuring and interfacial THz dynamics in setting cements. Materials Advances, 2022, 3, 4982-4990.	5.4	18
5	Ab initio random structure searching and catalytic properties of copper-based nanocluster with Earth-abundant metals for the electrocatalytic CO2-to-CO conversion. Molecular Catalysis, 2022, 527, 112406.	2.0	3
6	Iron porphyrin-derived ordered carbonaceous frameworks. Catalysis Today, 2021, 364, 164-171.	4.4	12
7	New insights into the role of solution additive anions in Mg²⁺ dehydration: implications for mineral carbonation. CrystEngComm, 2021, 23, 4896-4900.	2.6	18
8	Synthesis of graphene mesosponge via catalytic methane decomposition on magnesium oxide. Journal of Materials Chemistry A, 2021, 9, 14296-14308.	10.3	42
9	Endohedral Filling Effects in Sorted and Polymer-Wrapped Single-Wall Carbon Nanotubes. Journal of Physical Chemistry C, 2021, 125, 7476-7487.	3.1	8
10	Sulfate and Molybdate Incorporation at the Calciteâ€“Water Interface: Insights from Ab Initio Molecular Dynamics. ACS Earth and Space Chemistry, 2021, 5, 2066-2073.	2.7	3
11	The effect of the oxidation state of the metal center in metalloporphyrins on the electrocatalytic CO2-to-CO conversion: A density functional theory study. Molecular Catalysis, 2020, 498, 111248.	2.0	10
12	Hydrogenâ€Bond Structure and Lowâ€Frequency Dynamics of Electrolyte Solutions: Hydration Numbers from ab Initio Water Reorientation Dynamics and Dielectric Relaxation Spectroscopy. ChemPhysChem, 2020, 21, 2334-2346.	2.1	20
13	Density functional theory based molecular dynamics study of solution composition effects on the solvation shell of metal ions. Physical Chemistry Chemical Physics, 2020, 22, 16301-16313.	2.8	23
14	Interatomic potentials of Mg ions in aqueous solutions: structure and dehydration kinetics. European Journal of Mineralogy, 2019, 31, 275-287.	1.3	13
15	Reconsidering Calcium Dehydration as the Rate-Determining Step in Calcium Mineral Growth. Journal of Physical Chemistry C, 2019, 123, 26895-26903.	3.1	14
16	Solid and Aqueous Speciation of Yttrium in Passive Remediation Systems of Acid Mine Drainage. Environmental Science & Technology, 2019, 53, 11153-11161.	10.0	12
17	Prediction of self-assembly of adenosine analogues in solution: a computational approach validated by isothermal titration calorimetry. Physical Chemistry Chemical Physics, 2019, 21, 4258-4267.	2.8	9
18	The full dynamics of energy relaxation in large organic molecules: from photo-excitation to solvent heating. Chemical Science, 2019, 10, 4792-4804.	7.4	40

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19	Molecular modelling of the heat capacity and anisotropic thermal expansion of nanoporous hydroxyapatite. Materialia, 2019, 5, 100251.	2.7	13
20	Hydration numbers from ab initio water reorientation dynamics. , 2019, , .		0
21	Anomalous water and ion dynamics in hydroxyapatite mesopores. Computational Materials Science, 2019, 156, 26-34.	3.0	10
22	Water oxidation catalysed by quantum-sized BiVO₄. Journal of Materials Chemistry A, 2018, 6, 24965-24970.	10.3	10
23	Solvation and Aggregation of Meta-Aminobenzoic Acid in Water: Density Functional Theory and Molecular Dynamics Study. Pharmaceutics, 2018, 10, 12.	4.5	9
24	Role of Impurities in the Kinetic Persistence of Amorphous Calcium Carbonate: A Nanoscopic Dynamics View. Journal of Physical Chemistry C, 2018, 122, 16983-16991.	3.1	35
25	Transport properties of water molecules confined between hydroxyapaptite surfaces: A Molecular dynamics simulation approach. Applied Surface Science, 2017, 418, 296-301.	6.1	21
26	Detection of Posner's clusters during calcium phosphate nucleation: a molecular dynamics study. Journal of Materials Chemistry B, 2017, 5, 7274-7284.	5.8	50
27	Anisotropic diffusion of water molecules in hydroxyapatite nanopores. Physics and Chemistry of Minerals, 2017, 44, 509-519.	0.8	13
28	Is fast relaxation water really a free water?. , 2017, , .		1
29	Molecular Dynamics Simulations of Hydroxyapatite Nanopores in Contact with Electrolyte Solutions: The Effect of Nanoconfinement and Solvated Ions on the Surface Reactivity and the Structural, Dynamical, and Vibrational Properties of Water. Crystals, 2017, 7, 57.	2.2	19
30	Periodic vs. molecular cluster approaches to resolving glass structure and properties: Anorthite a case study. Journal of Non-Crystalline Solids, 2016, 451, 138-145.	3.1	20
31	Simulations reveal the role of composition into the atomic-level flexibility of bioactive glass cements. Physical Chemistry Chemical Physics, 2016, 18, 837-845.	2.8	14
32	The role of solvent in the self-assembly of m-aminobenzoic acid: a density functional theory and molecular dynamics study. CrystEngComm, 2016, 18, 2937-2948.	2.6	25
33	Properties of water confined in hydroxyapatite nanopores as derived from molecular dynamics simulations. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	22
34	Density Functional Theory Study of the Oligomerization of Carboxylic Acids. Journal of Physical Chemistry A, 2014, 118, 11098-11113.	2.5	27
35	Modelling the effects of salt solutions on the hydration of calcium ions. Physical Chemistry Chemical Physics, 2014, 16, 7772-7785.	2.8	54
36	Variations in calcite growth kinetics with surface topography: molecular dynamics simulations and process-based growth kinetics modelling. CrystEngComm, 2013, 15, 5506.	2.6	28

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37	The molecular self-association of carboxylic acids in solution: testing the validity of the link hypothesis using a quantum mechanical continuum solvation approach. CrystEngComm, 2013, 15, 6564.	2.6	44
38	Modelling the structural evolution of ternary phosphate glasses from melts to solid amorphous materials. Journal of Materials Chemistry B, 2013, 1, 5054.	5.8	23
39	Nanoscale Chains Control the Solubility of Phosphate Glasses for Biomedical Applications. Journal of Physical Chemistry B, 2013, 117, 10652-10657.	2.6	33
40	Density functional theory simulations of the structure, stability and dynamics of iron sulphide clusters in water. Physical Chemistry Chemical Physics, 2013, 15, 4310.	2.8	7
41	Calcite surface structure and reactivity: molecular dynamics simulations and macroscopic surface modelling of the calciteâ€“water interface. Physical Chemistry Chemical Physics, 2012, 14, 15145.	2.8	104
42	Polarizable force field development and molecular dynamics study of phosphate-based glasses. Journal of Chemical Physics, 2012, 137, 234502.	3.0	33
43	Density functional theory and interatomic potential study of structural, mechanical and surface properties of calcium oxalate materials. RSC Advances, 2012, 2, 4664.	3.6	22
44	The effects of ligand variation on enantioselective hydrogenation catalysed by RuH2(diphosphine)(diamine) complexes. Dalton Transactions, 2012, 41, 1867-1877.	3.3	14
45	Following the Creation of Active Gold Nanocatalysts from Phosphine-Stabilized Molecular Clusters. ACS Catalysis, 2012, 2, 957-963.	11.2	46
46	trans-FeII(H)2(diphosphine)(diamine) complexes as alternative catalysts for the asymmetric hydrogenation of ketones? A DFT study. Dalton Transactions, 2011, 40, 402-412.	3.3	28
47	Correlating Enantioselectivity with Activation Energies in the Asymmetric Hydrogenation of Acetophenone Catalysed by Noyori-Type Complexes. Catalysis Letters, 2011, 141, 1761-1766.	2.6	10
48	A density functional theory study of structural, mechanical and electronic properties of crystalline phosphorus pentoxide. Journal of Chemical Physics, 2011, 135, 234513.	3.0	14
49	An Ab Initio Molecular Dynamics Study of Bioactive Phosphate Glasses. Advanced Engineering Materials, 2010, 12, B331.	3.5	18
50	First Principles Simulations of the Structural and Dynamical Properties of Hydrated Metal Ions Me²⁺and Solvated Metal Carbonates (Me = Ca, Mg, and Sr). Crystal Growth and Design, 2010, 10, 4292-4302.	3.0	49
51	Interactions between Organophosphonate-Bearing Solutions and (101Ì…4) Calcite Surfaces: An Atomic Force Microscopy and First-Principles Molecular Dynamics Study. Crystal Growth and Design, 2010, 10, 3022-3035.	3.0	25
52	Structure and dynamics of the hydrated magnesium ion and of the solvated magnesium carbonates: insights from first principles simulations. Physical Chemistry Chemical Physics, 2010, 12, 894-901.	2.8	106
53	Accuracy of the microsolvationâ€“continuum approach in computing the pKa and the free energies of formation of phosphate species in aqueous solution. Physical Chemistry Chemical Physics, 2010, 12, 13804.	2.8	20
54	Conformational Effects in Photoelectron Circular Dichroism of Alaninol. ChemPhysChem, 2009, 10, 1839-1846.	2.1	45

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55	Theoretical study of the dimerization of calcium carbonate in aqueous solution under natural water conditions. Geochimica Et Cosmochimica Acta, 2009, 73, 5394-5405.	3.9	19
56	Hydrogen transfer and hydration properties of HnPO43â^'nâ€^(n=â€“3) in water studied by first principles molecular dynamics simulations. Journal of Chemical Physics, 2009, 130, 234502.	3.0	37
57	A Multilateral Mechanistic Study into Asymmetric Transfer Hydrogenation in Water. Chemistry - A European Journal, 2008, 14, 7699-7715.	3.3	194
58	The Onset of Calcium Carbonate Nucleation: A Density Functional Theory Molecular Dynamics and Hybrid Microsolvation/Continuum Study. Journal of Physical Chemistry B, 2008, 112, 6965-6975.	2.6	55
59	Computational Study of the Factors Controlling Enantioselectivity in Ruthenium(II) Hydrogenation Catalysts. Inorganic Chemistry, 2008, 47, 2674-2687.	4.0	40
60	New insights into the enantioselectivity in the hydrogenation of prochiral ketones. Chemical Communications, 2007, , 2381.	4.1	28
61	The H2-hydrogenation of ketones catalysed by ruthenium(II) complexes: A density functional theory study. Computational and Theoretical Chemistry, 2007, 812, 39-49.	1.5	33
62	Conformational Effects on Circular Dichroism in the Photoelectron Angular Distribution. ChemPhysChem, 2006, 7, 924-934.	2.1	46
63	Angle-Resolved Photoelectron Spectroscopy of Randomly Oriented 3-Hydroxytetrahydrofuran Enantiomers. ChemPhysChem, 2005, 6, 1164-1168.	2.1	33
64	Branching ratio deviations from statistical behavior in core photoionization. Journal of Chemical Physics, 2005, 123, 064311.	3.0	10