

Devis Di Tommaso

List of Publications by Year in descending order

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64
papers

1,769
citations

236925

25
h-index

302126

39
g-index

74
all docs

74
docs citations

74
times ranked

2208
citing authors

#	ARTICLE	IF	CITATIONS
1	A Multilateral Mechanistic Study into Asymmetric Transfer Hydrogenation in Water. Chemistry - A European Journal, 2008, 14, 7699-7715.	3.3	194
2	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
3	Calcite surface structure and reactivity: molecular dynamics simulations and macroscopic surface modelling of the calcite-water interface. Physical Chemistry Chemical Physics, 2012, 14, 15145.	2.8	104
4	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
5	Modelling the effects of salt solutions on the hydration of calcium ions. Physical Chemistry Chemical Physics, 2014, 16, 7772-7785.	2.8	54
6	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
7	First Principles Simulations of the Structural and Dynamical Properties of Hydrated Metal Ions Me^{2+} and Solvated Metal Carbonates (Me = Ca, Mg, and Sr). Crystal Growth and Design, 2010, 10, 4292-4302.	3.0	49
8	Conformational Effects on Circular Dichroism in the Photoelectron Angular Distribution. ChemPhysChem, 2006, 7, 924-934.	2.1	46
9	Following the Creation of Active Gold Nanocatalysts from Phosphine-Stabilized Molecular Clusters. ACS Catalysis, 2012, 2, 957-963.	11.2	46
10	Conformational Effects in Photoelectron Circular Dichroism of Alaninol. ChemPhysChem, 2009, 10, 1839-1846.	2.1	45
11	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
12	Synthesis of graphene mesosponge <i>via</i> catalytic methane decomposition on magnesium oxide. Journal of Materials Chemistry A, 2021, 9, 14296-14308.	10.3	42
13	Computational Study of the Factors Controlling Enantioselectivity in Ruthenium(II) Hydrogenation Catalysts. Inorganic Chemistry, 2008, 47, 2674-2687.	4.0	40
14	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
15	Hydrogen transfer and hydration properties of $HnPO_4^{3-n}$ ($n=3$) in water studied by first principles molecular dynamics simulations. Journal of Chemical Physics, 2009, 130, 234502.	3.0	37
16	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
17	Angle-Resolved Photoelectron Spectroscopy of Randomly Oriented 3-Hydroxytetrahydrofuran Enantiomers. ChemPhysChem, 2005, 6, 1164-1168.	2.1	33
18	The H ₂ -hydrogenation of ketones catalysed by ruthenium(II) complexes: A density functional theory study. Computational and Theoretical Chemistry, 2007, 812, 39-49.	1.5	33

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19	Polarizable force field development and molecular dynamics study of phosphate-based glasses. <i>Journal of Chemical Physics</i> , 2012, 137, 234502.	3.0	33
20	Nanoscale Chains Control the Solubility of Phosphate Glasses for Biomedical Applications. <i>Journal of Physical Chemistry B</i> , 2013, 117, 10652-10657.	2.6	33
21	New insights into the enantioselectivity in the hydrogenation of prochiral ketones. <i>Chemical Communications</i> , 2007, , 2381.	4.1	28
22	trans-Fell(H)2(diphosphine)(diamine) complexes as alternative catalysts for the asymmetric hydrogenation of ketones? A DFT study. <i>Dalton Transactions</i> , 2011, 40, 402-412.	3.3	28
23	Variations in calcite growth kinetics with surface topography: molecular dynamics simulations and process-based growth kinetics modelling. <i>CrystEngComm</i> , 2013, 15, 5506.	2.6	28
24	Density Functional Theory Study of the Oligomerization of Carboxylic Acids. <i>Journal of Physical Chemistry A</i> , 2014, 118, 11098-11113.	2.5	27
25	Interactions between Organophosphonate-Bearing Solutions and (101̄...4) Calcite Surfaces: An Atomic Force Microscopy and First-Principles Molecular Dynamics Study. <i>Crystal Growth and Design</i> , 2010, 10, 3022-3035.	3.0	25
26	The role of solvent in the self-assembly of m-aminobenzoic acid: a density functional theory and molecular dynamics study. <i>CrystEngComm</i> , 2016, 18, 2937-2948.	2.6	25
27	Modelling the structural evolution of ternary phosphate glasses from melts to solid amorphous materials. <i>Journal of Materials Chemistry B</i> , 2013, 1, 5054.	5.8	23
28	Density functional theory based molecular dynamics study of solution composition effects on the solvation shell of metal ions. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16301-16313.	2.8	23
29	Density functional theory and interatomic potential study of structural, mechanical and surface properties of calcium oxalate materials. <i>RSC Advances</i> , 2012, 2, 4664.	3.6	22
30	Properties of water confined in hydroxyapatite nanopores as derived from molecular dynamics simulations. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	1.4	22
31	Transport properties of water molecules confined between hydroxyapatite surfaces: A Molecular dynamics simulation approach. <i>Applied Surface Science</i> , 2017, 418, 296-301.	6.1	21
32	Accuracy of the microsolvation "continuum approach in computing the pKa and the free energies of formation of phosphate species in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 13804.	2.8	20
33	Periodic vs. molecular cluster approaches to resolving glass structure and properties: Anorthite a case study. <i>Journal of Non-Crystalline Solids</i> , 2016, 451, 138-145.	3.1	20
34	Hydrogen-Bond Structure and Low-Frequency Dynamics of Electrolyte Solutions: Hydration Numbers from ab Initio Water Reorientation Dynamics and Dielectric Relaxation Spectroscopy. <i>ChemPhysChem</i> , 2020, 21, 2334-2346.	2.1	20
35	Theoretical study of the dimerization of calcium carbonate in aqueous solution under natural water conditions. <i>Geochimica Et Cosmochimica Acta</i> , 2009, 73, 5394-5405.	3.9	19
36	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. <i>Crystals</i> , 2017, 7, 57.	2.2	19

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37	An Ab Initio Molecular Dynamics Study of Bioactive Phosphate Glasses. <i>Advanced Engineering Materials</i> , 2010, 12, B331.	3.5	18
38	New insights into the role of solution additive anions in Mg ²⁺ dehydration: implications for mineral carbonation. <i>CrystEngComm</i> , 2021, 23, 4896-4900.	2.6	18
39	Resolving nanoscopic structuring and interfacial THz dynamics in setting cements. <i>Materials Advances</i> , 2022, 3, 4982-4990.	5.4	18
40	A density functional theory study of structural, mechanical and electronic properties of crystalline phosphorus pentoxide. <i>Journal of Chemical Physics</i> , 2011, 135, 234513.	3.0	14
41	The effects of ligand variation on enantioselective hydrogenation catalysed by RuH ₂ (diphosphine)(diamine) complexes. <i>Dalton Transactions</i> , 2012, 41, 1867-1877.	3.3	14
42	Simulations reveal the role of composition into the atomic-level flexibility of bioactive glass cements. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 837-845.	2.8	14
43	Reconsidering Calcium Dehydration as the Rate-Determining Step in Calcium Mineral Growth. <i>Journal of Physical Chemistry C</i> , 2019, 123, 26895-26903.	3.1	14
44	Anisotropic diffusion of water molecules in hydroxyapatite nanopores. <i>Physics and Chemistry of Minerals</i> , 2017, 44, 509-519.	0.8	13
45	Interatomic potentials of Mg ions in aqueous solutions: structure and dehydration kinetics. <i>European Journal of Mineralogy</i> , 2019, 31, 275-287.	1.3	13
46	Molecular modelling of the heat capacity and anisotropic thermal expansion of nanoporous hydroxyapatite. <i>Materialia</i> , 2019, 5, 100251.	2.7	13
47	Solid and Aqueous Speciation of Yttrium in Passive Remediation Systems of Acid Mine Drainage. <i>Environmental Science & Technology</i> , 2019, 53, 11153-11161.	10.0	12
48	Iron porphyrin-derived ordered carbonaceous frameworks. <i>Catalysis Today</i> , 2021, 364, 164-171.	4.4	12
49	Branching ratio deviations from statistical behavior in core photoionization. <i>Journal of Chemical Physics</i> , 2005, 123, 064311.	3.0	10
50	Correlating Enantioselectivity with Activation Energies in the Asymmetric Hydrogenation of Acetophenone Catalysed by Noyori-Type Complexes. <i>Catalysis Letters</i> , 2011, 141, 1761-1766.	2.6	10
51	Water oxidation catalysed by quantum-sized BiVO ₄ . <i>Journal of Materials Chemistry A</i> , 2018, 6, 24965-24970.	10.3	10
52	Anomalous water and ion dynamics in hydroxyapatite mesopores. <i>Computational Materials Science</i> , 2019, 156, 26-34.	3.0	10
53	The effect of the oxidation state of the metal center in metalloporphyrins on the electrocatalytic CO ₂ -to-CO conversion: A density functional theory study. <i>Molecular Catalysis</i> , 2020, 498, 111248.	2.0	10
54	Solvation and Aggregation of Meta-Aminobenzoic Acid in Water: Density Functional Theory and Molecular Dynamics Study. <i>Pharmaceutics</i> , 2018, 10, 12.	4.5	9

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55	Prediction of self-assembly of adenosine analogues in solution: a computational approach validated by isothermal titration calorimetry. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 4258-4267.	2.8	9
56	Endohedral Filling Effects in Sorted and Polymer-Wrapped Single-Wall Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2021, 125, 7476-7487.	3.1	8
57	Porous nanographene formation on γ -alumina nanoparticles <i>via</i> transition-metal-free methane activation. <i>Chemical Science</i> , 2022, 13, 3140-3146.	7.4	8
58	Density functional theory simulations of the structure, stability and dynamics of iron sulphide clusters in water. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 4310.	2.8	7
59	A Database of Solution Additives Promoting Mg^{2+} Dehydration and the Onset of $MgCO_3$ Nucleation. <i>Crystal Growth and Design</i> , 2022, 22, 3080-3089.	3.0	5
60	Sulfate and Molybdate Incorporation at the Calcite-Water Interface: Insights from Ab Initio Molecular Dynamics. <i>ACS Earth and Space Chemistry</i> , 2021, 5, 2066-2073.	2.7	3
61	Ab initio random structure searching and catalytic properties of copper-based nanocluster with Earth-abundant metals for the electrocatalytic CO ₂ -to-CO conversion. <i>Molecular Catalysis</i> , 2022, 527, 112406.	2.0	3
62	Is fast relaxation water really a free water?. , 2017, , .		1
63	Bridging atomistic simulations and thermodynamic hydration models of aqueous electrolyte solutions. <i>Journal of Chemical Physics</i> , 2022, 156, 024502.	3.0	1
64	Hydration numbers from ab initio water reorientation dynamics. , 2019, , .		0