Daniel Sebastiani

List of Publications by Year
in descending order

146 papers	5,679 citations	87723 38 h-index	88477 70 g-index
152 all docs	152 docs citations	152 times ranked	6066 citing authors

#	Article	IF	Citations
1	Optimization of Effective Atom Centered Potentials for London Dispersion Forces in Density Functional Theory. Physical Review Letters, 2004, 93, 153004.	2.9	489
2	Isobaricâ^'Isothermal Molecular Dynamics Simulations Utilizing Density Functional Theory: An Assessment of the Structure and Density of Water at Near-Ambient Conditions. Journal of Physical Chemistry B, 2009, 113, 11959-11964.	1.2	327
3	A New ab-Initio Approach for NMR Chemical Shifts in Periodic Systems. Journal of Physical Chemistry A, 2001, 105, 1951-1958.	1.1	207
4	Generalized variational density functional perturbation theory. Journal of Chemical Physics, 2000, 113, 7102-7109.	1.2	183
5	Mixed Grotthuss and Vehicle Transport Mechanism in Proton Conducting Polymers from Ab initio Molecular Dynamics Simulations. Chemistry of Materials, 2011, 23, 1424-1429.	3.2	172
6	High-Resolution Solid-State NMR Studies of Imidazole-Based Proton Conductors:â€‰ Structure Motifs and Chemical Exchange from 1H NMR. Journal of Physical Chemistry B, 2002, 106, 9322-9334.	1.2	164
7	A Strategy for Revealing the Packing in Semicrystalline Ï€â€Conjugated Polymers: Crystal Structure of Bulk Polyâ€3â€hexylâ€thiophene (P3HT). Angewandte Chemie - International Edition, 2012, 51, 11068-11072.	7.2	160
8	Annularly Fused Hexapyrrolohexaazacoronenes: An Extended Ï€â€...System with Multiple Interior Nitrogen Atoms Displays Stable Oxidation States. Angewandte Chemie - International Edition, 2007, 46, 5524-5527.	7.2	154
9	From Armchair to Zigzag Peripheries in Nanographenes. Journal of the American Chemical Society, 2006, 128, 9526-9534.	6.6	153
10	High-Resolution Solid-State NMR Studies of Poly(vinyl phosphonic acid) Proton-Conducting Polymer:â€‰ Molecular Structure and Proton Dynamics. Journal of Physical Chemistry B, 2007, 111, 9711-9721.	1.2	138
11	Ab Initio Molecular Dynamics-Based Assignment of the Protonation State of Pepstatin A/HIV-1 Protease Cleavage Site. Journal of the American Chemical Society, 2001, 123, 8730-8737.	6.6	124
12	Self-Assembly of Dendronized Perylene Bisimides into Complex Helical Columns. Journal of the American Chemical Society, 2011, 133, 12197-12219.	6.6	120
13	Benzoxazine Oligomers:Â Evidence for a Helical Structure from Solid-State NMR Spectroscopy and DFT-Based Dynamics and Chemical Shift Calculations. Journal of the American Chemical Society, 2003, 125, 5792-5800.	6.6	116
14	Variational optimization of effective atom centered potentials for molecular properties. Journal of Chemical Physics, 2005, 122, 014113.	1.2	110
15	Performance of optimized atom-centered potentials for weakly bonded systems using density functional theory. Physical Review B, 2005, 71, .	1.1	107
16	Supramolecular Assembly of Dendritic Polymers Elucidated by1H and13C Solid-State MAS NMR Spectroscopy. Journal of the American Chemical Society, 2003, 125, 13284-13297.	6.6	106
17	Bulk Chemical Shifts in Hydrogen-Bonded Systems from First-Principles Calculations and Solid-State-NMR. Journal of Physical Chemistry B, 2006, 110, 23204-23210.	1.2	94
18	Current Densities and Nucleus-Independent Chemical Shift Maps from Reciprocal-Space Density Functional Perturbation Theory Calculations. ChemPhysChem, 2006, 7, 164-175.	1.0	89

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19	Empty Helical Nanochannels with Adjustable Order from Lowâ€Symmetry Macrocycles. Angewandte Chemie - International Edition, 2011, 50, 3030-3033.	7.2	79
20	Columnar Packing Motifs of Functionalized Perylene Derivatives: Local Molecular Order Despite Long-Range Disorder. Journal of the American Chemical Society, 2009, 131, 5251-5256.	6.6	71
21	Nuclear velocity perturbation theory for vibrational circular dichroism: An approach based on the exact factorization of the electron-nuclear wave function. Journal of Chemical Physics, 2015, 143, 074106.	1.2	67
22	Proton momentum distribution in water: an open path integral molecular dynamics study. Journal of Chemical Physics, 2007, 126, 234504.	1.2	66
23	Ab-initio Study of NMR Chemical Shifts of Water Under Normal and Supercritical Conditions. ChemPhysChem, 2002, 3, 675.	1.0	65
24	Adsorption of Water Molecules on Flat and Stepped Nickel Surfaces from First Principles. Journal of Chemical Theory and Computation, 2005, 1, 78-82.	2.3	64
25	2H Solid-State NMR of Mobile Protons:Â It Is Not Always the Simple Way. Journal of the American Chemical Society, 2007, 129, 12406-12407.	6.6	62
26	Nuclear Magnetic Resonance Chemical Shifts from Hybrid DFT QM/MM Calculations. Journal of Physical Chemistry B, 2004, 108, 2807-2815.	1.2	58
27	Mechanism for the Stable Performance of Sulfur-Copolymer Cathode in Lithiumâ€“Sulfur Battery Studied by Solid-State NMR Spectroscopy. Chemistry of Materials, 2018, 30, 2915-2923.	3.2	58
28	Electronic Response Properties of Carbon Nanotubes in Magnetic Fields. ACS Nano, 2008, 2, 661-668.	7.3	57
29	Vibrational circular dichroism from ab initio molecular dynamics and nuclear velocity perturbation theory in the liquid phase. Journal of Chemical Physics, 2016, 145, 084101.	1.2	53
30	Chiral Crystal Packing Induces Enhancement of Vibrational Circular Dichroism. Angewandte Chemie - International Edition, 2018, 57, 13344-13348.	7.2	51
31	Nuclear Velocity Perturbation Theory of Vibrational Circular Dichroism. Journal of Chemical Theory and Computation, 2013, 9, 5305-5312.	2.3	49
32	Low temperature annealing in tetrahedral amorphous carbon thin films observed by13CNMR spectroscopy. Physical Review B, 2003, 67, .	1.1	47
33	NMR chemical shifts in periodic systems from first principles. Computer Physics Communications, 2002, 147, 707-710.	3.0	45
34	Molecular Mechanism of Overhauser Dynamic Nuclear Polarization in Insulating Solids. Journal of Physical Chemistry Letters, 2017, 8, 2137-2142.	2.1	44
35	First Principles and Experimental 1H NMR Signatures of Solvated Ions: The Case of HCl(aq). ChemPhysChem, 2006, 7, 2578-2584.	1.0	43
36	Triazolium-Based Ionic Liquids: A Novel Class of Cellulose Solvents. Journal of Physical Chemistry B, 2019, 123, 3994-4003.	1.2	43

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37	NMR Chemical Shifts of the Rhodopsin Chromophore in the Dark State and in Bathorhodopsin:Â A Hybrid QM/MM Molecular Dynamics Study. Journal of Physical Chemistry B, 2008, 112, 1267-1274.	1.2	42
38	Salt Bridge in Aqueous Solution: Strong Structural Motifs but Weak Enthalpic Effect. Scientific Reports, 2018, 8, 13626.	1.6	41
39	The impact of the amide connectivity on the assembly and dynamics of benzene-1,3,5-tricarboxamides in the solid state. Chemical Science, 2011, 2, 2040.	3.7	39
40	Local Microphase Separation of a Binary Liquid under Nanoscale Confinement. Journal of Physical Chemistry B, 2014, 118, 10207-10213.	1.2	39
41	Water and small organic molecules as probes for geometric confinement in well-ordered mesoporous carbon materials. Physical Chemistry Chemical Physics, 2014, 16, 9327-9336.	1.3	36
42	Polar solvent fluctuations drive proton transfer in hydrogen bonded complexes of carboxylic acid with pyridines: NMR, IR and ab initio MD study. Physical Chemistry Chemical Physics, 2017, 19, 1010-1028.	1.3	35
43	NMR Solvent Shifts of Adenine in Aqueous Solution from Hybrid QM/MM Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2007, 111, 5225-5232.	1.2	34
44	Solvent molecules trapped in supramolecular organic nanotubes: a combined solid-state NMR and DFT study. Chemical Physics Letters, 2004, 388, 164-169.	1.2	32
45	AB-INITIO CALCULATIONS OF NMR PARAMETERS IN CONDENSED PHASES. Modern Physics Letters B, 2003, 17, 1301-1319.	1.0	31
46	Diffusion in binary gas mixtures studied by NMR of hyperpolarized gases and molecular dynamics simulations. Physical Chemistry Chemical Physics, 2006, 8, 4182-4188.	1.3	31
47	Proton transfer in a short hydrogen bond caused by solvation shell fluctuations: an ab initio MD and NMR/UV study of an (OHO)^{â^'} bonded system. Physical Chemistry Chemical Physics, 2015, 17, 4634-4644.	1.3	29
48	Improved Quantum Chemical NMR Chemical Shift Prediction of Metabolites in Aqueous Solution toward the Validation of Unknowns. Journal of Physical Chemistry A, 2017, 121, 3071-3078.	1.1	29
49	NMR chemical shifts in proton conducting crystals from first principles. Computational and Theoretical Chemistry, 2003, 625, 283-288.	1.5	28
50	Selectivity of guestâ€“host interactions in self-assembled hydrogen-bonded nanostructures observed by NMR. Physical Chemistry Chemical Physics, 2007, 9, 4545.	1.3	28
51	Beyond Isotropic Tumbling Models: Nuclear Spin Relaxation in Liquids from First Principles. ChemPhysChem, 2008, 9, 2313-2316.	1.0	28
52	Vibrational Frequencies of Water Adsorbed on (111) and (221) Nickel Surfaces from First Principle Calculations. ChemPhysChem, 2006, 7, 1215-1219.	1.0	27
53	On the Mass of Atoms in Molecules: Beyond the Born-Oppenheimer Approximation. Physical Review X, 2017, 7, .	2.8	26
54	Ultrafast Proton Transport between a Hydroxy Acid and a Nitrogen Base along Solvent Bridges Governed by the Hydroxide/Methoxide Transfer Mechanism. Journal of the American Chemical Society, 2019, 141, 14581-14592.	6.6	26

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55	NMR chemical shifts as a tool to analyze first principles molecular dynamics simulations in condensed phases: the case of liquid water. Magnetic Resonance in Chemistry, 2010, 48, S56-S60.	1.1	25
56	Accurate Total Energies without Self-Consistency. Physical Review Letters, 2001, 87, 226401.	2.9	24
57	Artificial Bee Colony Optimization of Capping Potentials for Hybrid Quantum Mechanical/Molecular Mechanical Calculations. Journal of Chemical Theory and Computation, 2011, 7, 1307-1315.	2.3	24
58	Effect of puckering motion and hydrogen bond formation on the vibrational circular dichroism spectrum of a flexible molecule: the case of (S)-1-indanol. Physical Chemistry Chemical Physics, 2018, 20, 14635-14646.	1.3	24
59	Anomalous temperature dependence of nuclear quadrupole interactions in strongly hydrogen-bonded systems from first principles. Journal of Chemical Physics, 2005, 123, 074501.	1.2	23
60	Symmetry and dynamics of FHF^{â^'} anion in vacuum, in CD₂Cl₂ and in CCl₄. Ab initio MD study of fluctuating solventâ€“solute hydrogen and halogen bonds. Physical Chemistry Chemical Physics, 2017, 19, 26107-26120.	1.3	23
61	Dissolving Cellulose in 1,2,3-Triazolium- and Imidazolium-Based Ionic Liquids with Aromatic Anions. Molecules, 2020, 25, 3539.	1.7	23
62	Is NMR the tool to characterize the structure of C20 isomers?. Chemical Physics Letters, 2002, 366, 134-140.	1.2	22
63	Local Disorder in Hydrogen Storage Compounds: The Case of Lithium Amide/Imide. ChemPhysChem, 2010, 11, 2353-2360.	1.0	22
64	Visualizing Degrees of Aromaticity for Different Barbaralane Systems. Journal of Physical Chemistry A, 2004, 108, 11728-11732.	1.1	21
65	An Ab Initio Microscope: Molecular Contributions to the Femtosecond Timeâ€Dependent Fluorescence Shift of a Reichardtâ€Type Dye. Angewandte Chemie - International Edition, 2013, 52, 1813-1816.	7.2	21
66	Ab Initio H₂O in Realistic Hydrophilic Confinement. ChemPhysChem, 2014, 15, 3955-3962.	1.0	21
67	Competition between excited state proton and OH^{â^'} transport via a short water wire: solvent effects open the gate. Physical Chemistry Chemical Physics, 2014, 16, 13047-13051.	1.3	21
68	Structural heterogeneity in a parent ground-state structure of AnPixJg2 revealed by theory and spectroscopy. Physical Chemistry Chemical Physics, 2017, 19, 13882-13894.	1.3	21
69	H-Bonding Competition and Clustering in Aqueous LiI. Journal of Physical Chemistry B, 2013, 117, 9939-9946.	1.2	20
70	A Coupled Molecular Dynamics/Kinetic Monte Carlo Approach for Protonation Dynamics in Extended Systems. Journal of Chemical Theory and Computation, 2014, 10, 4221-4228.	2.3	19
71	Simulating structure and dynamics in small droplets of 1-ethyl-3-methylimidazolium acetate. Journal of Chemical Physics, 2018, 148, 193802.	1.2	19
72	Specific quantum mechanical/molecular mechanical capping-potentials for biomolecular functional groups. Journal of Chemical Physics, 2011, 135, 214107.	1.2	18

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73	Water Wires in Aqueous Solutions from First-Principles Calculations. Journal of Physical Chemistry B, 2015, 119, 4053-4060.	1.2	18
74	The structure and IR signatures of the arginine-glutamate salt bridge. Insights from the classical MD simulations. Journal of Chemical Physics, 2015, 142, 215106.	1.2	18
75	Effect of a step defect on the adsorption of benzene on the (221) surface of nickel:â€ƒAnab initiostudy. Physical Review B, 2004, 70, .	1.1	17
76	Optimization of Capping Potentials for Spectroscopic Parameters in Hybrid Quantum Mechanical/Mechanical Modeling Calculations. Journal of Chemical Theory and Computation, 2009, 5, 1490-1498.	2.3	17
77	Combined Experimental and Theoretical Study of the Transient IR Spectroscopy of 7-Hydroxyquinoline in the First Electronically Excited Singlet State. Journal of Physical Chemistry A, 2016, 120, 9378-9389.	1.1	17
78	Approaches to the solvation of the molecular probe N-methyl-6-quinolone in its excited state. Physical Chemistry Chemical Physics, 2011, 13, 16395.	1.3	16
79	Water-Free Proton Conduction in Hexakis(p-Phosphonatophenyl)benzene Nanochannels. Journal of Physical Chemistry C, 2013, 117, 12366-12372.	1.5	16
80	Liquid Water Confined in Cellulose with Variable Interfacial Hydrophilicity. Zeitschrift Fur Physikalische Chemie, 2018, 232, 989-1002.	1.4	16
81	Solid-state NMR and computational studies of tetratolyl urea calix[4]arene inclusion compounds. Physical Chemistry Chemical Physics, 2009, 11, 9241.	1.3	15
82	Dinitrogen complexation with main group radicals. Chemical Science, 2011, 2, 473-479.	3.7	15
83	The important role of non-covalent interactions for the vibrational circular dichroism of lactic acid in aqueous solution. Physical Chemistry Chemical Physics, 2021, 23, 17232-17241.	1.3	15
84	Solvation of Small Disulfonate Anions in Water/Methanol Mixtures Characterized by High-Field Pulse Electron Nuclear Double Resonance and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 7429-7438.	1.2	14
85	Phycocyanobilin in solution â€“ a solvent triggered molecular switch. Physical Chemistry Chemical Physics, 2014, 16, 6146-6152.	1.3	14
86	Perturbation of the F19-L34 Contact in Amyloid Î² (1-40) Fibrils Induces Only Local Structural Changes but Abolishes Cytotoxicity. Journal of Physical Chemistry Letters, 2017, 8, 4740-4745.	2.1	14
87	The Isotope-Effect in the Phase Transition of KH2PO4: New Insights from Ab Initio Path-Integral Simulations. Journal of Physical Chemistry C, 2011, 115, 12631-12635.	1.5	13
88	A Generalized Packing Model for Bulk Crystalline Regioregular Poly(3â€alkylthiophenes) with Extended Side Chains. Macromolecular Chemistry and Physics, 2018, 219, 1700266.	1.1	12
89	First Principles Calculations of NMR Chemical Shifts of Liquid Water at an Amorphous Silica Interface. Zeitschrift Fur Physikalische Chemie, 2012, 226, 1415-1424.	1.4	11
90	Unraveling the existence of dynamic water channels in light-harvesting proteins: alpha-C-phycocyanobilin in vitro. Chemical Science, 2013, 4, 755-763.	3.7	11

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91	Methyl rotor quantum states and the effect of chemical environment in organic crystals: Î³-picoline and toluene. Journal of Chemical Physics, 2016, 145, 234506.	1.2	11
92	Proton Conductivity in Hydrogen Phosphate/Sulfates from a Coupled Molecular Dynamics/Lattice Monte Carlo (cMD/LMC) Approach. Journal of Physical Chemistry C, 2016, 120, 19913-19922.	1.5	11
93	Tunneling of coupled methyl quantum rotors in 4-methylpyridine: Single rotor potential versus coupling interaction. Journal of Chemical Physics, 2017, 147, 194303.	1.2	11
94	Reply to Comment on â€œMixed Grotthuss and Vehicle Transport Mechanism in Proton Conducting Polymers from Ab initio Molecular Dynamics Simulationsâ€. Chemistry of Materials, 2011, 23, 3379-3380.	3.2	10
95	Hydrogen bond networks: Structure and dynamics via firstâ€principles spectroscopy. Physica Status Solidi (B): Basic Research, 2012, 249, 368-375.	0.7	10
96	Perfluoroalkane Force Field for Lipid Membrane Environments. Journal of Physical Chemistry B, 2014, 118, 12531-12540.	1.2	10
97	Switching between Proton Vacancy and Excess Proton Transfer Pathways in the Reaction between 7-Hydroxyquinoline and Formate. Journal of Physical Chemistry A, 2021, 125, 1845-1859.	1.1	10
98	On the Structure of Sulfur/1,3â€Diisopropenylbenzene Coâ€Polymer Cathodes for Liâ€S Batteries: Insights from Densityâ€Functional Theory Calculations. ChemPhysChem, 2022, 23, .	1.0	10
99	Molecular Mechanisms of Additive Fortification in Model Epoxy Resins: A Solid State NMR Study. Macromolecules, 2010, 43, 7200-7211.	2.2	9
100	Eigensystem Representation of the Electronic Susceptibility Tensor for Intermolecular Interactions within Density Functional Theory. Journal of Chemical Theory and Computation, 2012, 8, 106-111.	2.3	9
101	Mechanism of ion conductivity through polymer-stabilized CsH₂PO₄ nanoparticular layers from experiment and theory. Journal of Materials Chemistry A, 2019, 7, 27367-27376.	5.2	9
102	Polyhedral Phenylacetylenes: The Interplay of Aromaticity and Antiaromaticity in Convex Graphyne Substructures. Symmetry, 2009, 1, 226-239.	1.1	8
103	Foraging on the potential energy surface: A swarm intelligence-based optimizer for molecular geometry. Journal of Chemical Physics, 2012, 137, 194110.	1.2	8
104	Toward Realistic Transfer Rates within the Coupled Molecular Dynamics/Lattice Monte Carlo Approach. Journal of Physical Chemistry C, 2016, 120, 19905-19912.	1.5	8
105	The annular tautomerism of lithium 1,2,3-triazolate. New Journal of Chemistry, 2017, 41, 1430-1435.	1.4	8
106	Proton mobility in aqueous systems: combining ab initio accuracy with millisecond timescales. Physical Chemistry Chemical Physics, 2017, 19, 28604-28609.	1.3	8
107	Effect of anion reorientation on proton mobility in the solid acids family CsH_yXO₄(X = S, P, Se,y= 1, 2) fromab initiomolecular dynamics simulations. Physical Chemistry Chemical Physics, 2020, 22, 10738-10752.	1.3	8
108	Possibility of Coherent Delocalized Nuclear Quantum States of Protons in Li₂NH. Journal of Physical Chemistry Letters, 2010, 1, 3214-3218.	2.1	7

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109	Electronic density response to molecular geometric changes from explicit electronic susceptibility calculations. Journal of Chemical Physics, 2013, 139, 094102.	1.2	7
110	Linear Response Methods in Quantum Chemistry. Letters in Mathematical Physics, 2014, , 97-110.	0.4	7
111	Solvation-Dependent Latency of Photoacid Dissociation and Transient IR Signatures of Protonation Dynamics. Journal of Physical Chemistry A, 2015, 119, 9244-9251.	1.1	7
112	Dynamical Dimension to the Hofmeister Series: Insights from Firstâ€Principles Simulations. ChemPhysChem, 2016, 17, 1166-1173.	1.0	7
113	Local Disorder in Lithium Imide from Density Functional Simulation and NMR Spectroscopy. Journal of Physical Chemistry C, 2012, 116, 18577-18583.	1.5	6
114	First principles calculation of inhomogeneous broadening in solid-state cw-EPR spectroscopy. Physical Chemistry Chemical Physics, 2013, 15, 16082.	1.3	6
115	Moment expansion of the linear densityâ€density response function. Journal of Computational Chemistry, 2016, 37, 665-674.	1.5	6
116	Dynamical matrix propagator scheme for large-scale proton dynamics simulations. Journal of Chemical Physics, 2020, 152, 114114.	1.2	6
117	Insight from Atomistic Simulations of Protonation Dynamics at the Nanoscale. Fuel Cells, 2016, 16, 682-694.	1.5	5
118	Influence of Small Fluorophilic and Lipophilic Organic Molecules on Dipalmitoylphosphatidylcholine Bilayers. Journal of Physical Chemistry B, 2017, 121, 8311-8321.	1.2	5
119	Ab-Initio Molecular Dynamics Simulations and Calculations of Spectroscopic Parameters in Hydrogen-Bonding Liquids in Confinement (Project 8). Zeitschrift Fur Physikalische Chemie, 2018, 232, 973-987.	1.4	5
120	Carbon Atoms Speaking Out: How the Geometric Sensitivity of 13C Chemical Shifts Leads to Understanding the Colour Tuning of Phycocyanobilin in Cph1 and AnPixJ. Molecules, 2020, 25, 5505.	1.7	5
121	Exploring non-equilibrium molecular dynamics of mobile protons in the solid acid CsH2PO4 at the micrometer and microsecond scale. Journal of Chemical Physics, 2020, 152, 164110.	1.2	5
122	Hydrogen Bond between a Tyrosine Residue and the C-Ring Propionate Has a Direct Influence on Conformation and Absorption of the Bilin Cofactor in Red/Green Cyanobacteriochromes. Journal of Physical Chemistry B, 2021, 125, 1331-1342.	1.2	5
123	Conformational Space of a Polyphilic Molecule with a Fluorophilic Side Chain Integrated in a DPPC Bilayer. Journal of Computational Chemistry, 2017, 38, 576-583.	1.5	4
124	VCDâ€VerstÃrkung durch chirale Packungseffekte in molekularen Kristallen. Angewandte Chemie, 2018, 130, 13528-13532.	1.6	4
125	Iterative approach for the moment representation of the density-density response function. European Physical Journal B, 2018, 91, 1.	0.6	4
126	Efficient representation of the linear densityâ€density response function. Journal of Computational Chemistry, 2019, 40, 2712-2721.	1.5	4

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127	From flat to tilted: gradual interfaces in organic thin film growth. Nanoscale, 2020, 12, 3834-3845.	2.8	4
128	Gold diggers: Altered reconstruction of the gold surface by physisorbed aromatic oligomers. Physical Review Materials, 2019, 3, .	0.9	4
129	The relation between crystal structure and the occurrence of quantum-rotor-induced polarization. Magnetic Resonance, 2021, 2, 751-763.	0.8	4
130	Crystalline diamond polymorphs analyzed with first-principles13C NMR chemical shift calculations. International Journal of Quantum Chemistry, 2005, 101, 849-853.	1.0	3
131	Efficient implementation and application of the artificial bee colony algorithm to low-dimensional optimization problems. Computer Physics Communications, 2014, 185, 1639-1646.	3.0	3
132	Generalization of the electronic susceptibility for arbitrary molecular geometries. Journal of Chemical Physics, 2016, 144, 144111.	1.2	3
133	The Conformational Ensemble of Polyglutamineâ€14 Chains: Specific Influences of Solubility Tail and Chromophores. ChemPhysChem, 2018, 19, 2931-2937.	1.0	3
134	ab-Initio Study of Hydrogen Bond Networks in 1,2,3-Triazole Phases. Molecules, 2020, 25, 5722.	1.7	3
135	Advances in Density-functional-based Modeling Techniques - Recent Extensions of the Car-Parrinello Approach. Methods and Principles in Medicinal Chemistry, 2005, , 3-39.	0.3	2
136	Spectroscopic fingerprints of toroidal nuclear quantum delocalization via ab initio path integral simulations. Journal of Computational Chemistry, 2013, 34, 827-835.	1.5	2
137	Mechanism of Lithium Cation Hopping between Tetragonal Thiophene Cages. Batteries and Supercaps, 2019, 2, 695-700.	2.4	2
138	Reduced eigensystem representation of the linear densityâ€density response function. International Journal of Quantum Chemistry, 2020, 120, e26085.	1.0	2
139	Optimized effective potentials to increase the accuracy of approximate proton transfer energy calculations in the excited state. Journal of Chemical Physics, 2020, 152, 064101.	1.2	2
140	Cluster Formation of Polyphilic Molecules Solvated in a DPPC Bilayer. Polymers, 2017, 9, 488.	2.0	1
141	Polyphilic Interactions as Structural Driving Force Investigated by Molecular Dynamics Simulation (Project 7). Polymers, 2017, 9, 445.	2.0	1
142	Ultrafast proton transport in water-methanol mixtures. EPJ Web of Conferences, 2019, 205, 09004.	0.1	1
143	Polarization Energies from Efficient Representation of the Linear Densityâ€“Density Response Function. Advanced Theory and Simulations, 2021, 4, 2000260.	1.3	1
144	Atomistic Diffusion Pathways of Lithium Ions in Crystalline Lithium Silicides from ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry C, 0, , .	1.5	1

#	Article	IF	Citations
145	RÃ¼cktitelbild: VCDâ€VerstÃrkung durch chirale Packungseffekte in molekularen Kristallen (Angew.) Tj ETQq1 1 0.784314 rgBT /Ove	1.6	0
146	Minimal Optimized Effective Potentials for Density Functional Theory Studies on Excited-State Proton Dissociation. Micromachines, 2021, 12, 679.	1.4	0