Daniel Sebastiani

List of Publications by Year
in descending order

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146 papers	5,679 citations	87843 38 h-index	88593 70 g-index
152 all docs	152 docs citations	152 times ranked	6066 citing authors

#	Article	IF	Citations
1	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
2	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
3	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
4	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
5	Minimal Optimized Effective Potentials for Density Functional Theory Studies on Excited-State Proton Dissociation. Micromachines, 2021, 12, 679.	1.4	0
6	Polarization Energies from Efficient Representation of the Linear Densityâ€“Density Response Function. Advanced Theory and Simulations, 2021, 4, 2000260.	1.3	1
7	The relation between crystal structure and the occurrence of quantum-rotor-induced polarization. Magnetic Resonance, 2021, 2, 751-763.	0.8	4
8	Reduced eigensystem representation of the linear densityâ€density response function. International Journal of Quantum Chemistry, 2020, 120, e26085.	1.0	2
9	Dissolving Cellulose in 1,2,3-Triazolium- and Imidazolium-Based Ionic Liquids with Aromatic Anions. Molecules, 2020, 25, 3539.	1.7	23
10	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
11	ab-Initio Study of Hydrogen Bond Networks in 1,2,3-Triazole Phases. Molecules, 2020, 25, 5722.	1.7	3
12	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
13	Dynamical matrix propagator scheme for large-scale proton dynamics simulations. Journal of Chemical Physics, 2020, 152, 114114.	1.2	6
14	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
15	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
16	From flat to tilted: gradual interfaces in organic thin film growth. Nanoscale, 2020, 12, 3834-3845.	2.8	4
17	Efficient representation of the linear densityâ€density response function. Journal of Computational Chemistry, 2019, 40, 2712-2721.	1.5	4
18	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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19	Ultrafast proton transport in water-methanol mixtures. EPJ Web of Conferences, 2019, 205, 09004.	0.1	1
20	Mechanism of Lithium Cation Hopping between Tetragonal Thiophene Cages. Batteries and Supercaps, 2019, 2, 695-700.	2.4	2
21	Triazolium-Based Ionic Liquids: A Novel Class of Cellulose Solvents. Journal of Physical Chemistry B, 2019, 123, 3994-4003.	1.2	43
22	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
23	Gold diggers: Altered reconstruction of the gold surface by physisorbed aromatic oligomers. Physical Review Materials, 2019, 3, .	0.9	4
24	Simulating structure and dynamics in small droplets of 1-ethyl-3-methylimidazolium acetate. Journal of Chemical Physics, 2018, 148, 193802.	1.2	19
25	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
26	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
27	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
28	Liquid Water Confined in Cellulose with Variable Interfacial Hydrophilicity. Zeitschrift Fur Physikalische Chemie, 2018, 232, 989-1002.	1.4	16
29	RÃ¼cktitelbild: VCDâ€VerstÃrkung durch chirale Packungseffekte in molekularen Kristallen (Angew.) Tj ETQq1 1 0.784314 rgBT /Ove	1.6	0
30	VCDâ€VerstÃrkung durch chirale Packungseffekte in molekularen Kristallen. Angewandte Chemie, 2018, 130, 13528-13532.	1.6	4
31	Salt Bridge in Aqueous Solution: Strong Structural Motifs but Weak Enthalpic Effect. Scientific Reports, 2018, 8, 13626.	1.6	41
32	Chiral Crystal Packing Induces Enhancement of Vibrational Circular Dichroism. Angewandte Chemie - International Edition, 2018, 57, 13344-13348.	7.2	51
33	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
34	The Conformational Ensemble of Polyglutamineâ€14 Chains: Specific Influences of Solubility Tail and Chromophores. ChemPhysChem, 2018, 19, 2931-2937.	1.0	3
35	Iterative approach for the moment representation of the density-density response function. European Physical Journal B, 2018, 91, 1.	0.6	4
36	The annular tautomerism of lithium 1,2,3-triazolate. New Journal of Chemistry, 2017, 41, 1430-1435.	1.4	8

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37	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
38	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
39	Molecular Mechanism of Overhauser Dynamic Nuclear Polarization in Insulating Solids. Journal of Physical Chemistry Letters, 2017, 8, 2137-2142.	2.1	44
40	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
41	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
42	Proton mobility in aqueous systems: combining ab initio accuracy with millisecond timescales. Physical Chemistry Chemical Physics, 2017, 19, 28604-28609.	1.3	8
43	On the Mass of Atoms in Molecules: Beyond the Born-Oppenheimer Approximation. Physical Review X, 2017, 7, .	2.8	26
44	Influence of Small Fluorophilic and Lipophilic Organic Molecules on Dipalmitoylphosphatidylcholine Bilayers. Journal of Physical Chemistry B, 2017, 121, 8311-8321.	1.2	5
45	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
46	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
47	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
48	Cluster Formation of Polyphilic Molecules Solvated in a DPPC Bilayer. Polymers, 2017, 9, 488.	2.0	1
49	Polyphilic Interactions as Structural Driving Force Investigated by Molecular Dynamics Simulation (Project 7). Polymers, 2017, 9, 445.	2.0	1
50	Dynamical Dimension to the Hofmeister Series: Insights from Firstâ€Principles Simulations. ChemPhysChem, 2016, 17, 1166-1173.	1.0	7
51	Generalization of the electronic susceptibility for arbitrary molecular geometries. Journal of Chemical Physics, 2016, 144, 144111.	1.2	3
52	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
53	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
54	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

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55	Insight from Atomistic Simulations of Protonation Dynamics at the Nanoscale. Fuel Cells, 2016, 16, 682-694.	1.5	5
56	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
57	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
58	Moment expansion of the linear densityâ€density response function. Journal of Computational Chemistry, 2016, 37, 665-674.	1.5	6
59	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
60	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
61	Water Wires in Aqueous Solutions from First-Principles Calculations. Journal of Physical Chemistry B, 2015, 119, 4053-4060.	1.2	18
62	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
63	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
64	Ab Initio H₂O in Realistic Hydrophilic Confinement. ChemPhysChem, 2014, 15, 3955-3962.	1.0	21
65	Linear Response Methods in Quantum Chemistry. Letters in Mathematical Physics, 2014, , 97-110.	0.4	7
66	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
67	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
68	Perfluoroalkane Force Field for Lipid Membrane Environments. Journal of Physical Chemistry B, 2014, 118, 12531-12540.	1.2	10
69	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
70	Local Microphase Separation of a Binary Liquid under Nanoscale Confinement. Journal of Physical Chemistry B, 2014, 118, 10207-10213.	1.2	39
71	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
72	Phycocyanobilin in solution â€“ a solvent triggered molecular switch. Physical Chemistry Chemical Physics, 2014, 16, 6146-6152.	1.3	14

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73	H-Bonding Competition and Clustering in Aqueous LiI. Journal of Physical Chemistry B, 2013, 117, 9939-9946.	1.2	20
74	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
75	First principles calculation of inhomogeneous broadening in solid-state cw-EPR spectroscopy. Physical Chemistry Chemical Physics, 2013, 15, 16082.	1.3	6
76	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
77	Water-Free Proton Conduction in Hexakis(p-Phosphonatophenyl)benzene Nanochannels. Journal of Physical Chemistry C, 2013, 117, 12366-12372.	1.5	16
78	Nuclear Velocity Perturbation Theory of Vibrational Circular Dichroism. Journal of Chemical Theory and Computation, 2013, 9, 5305-5312.	2.3	49
79	Electronic density response to molecular geometric changes from explicit electronic susceptibility calculations. Journal of Chemical Physics, 2013, 139, 094102.	1.2	7
80	Spectroscopic fingerprints of toroidal nuclear quantum delocalization via ab initio path integral simulations. Journal of Computational Chemistry, 2013, 34, 827-835.	1.5	2
81	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
82	Foraging on the potential energy surface: A swarm intelligence-based optimizer for molecular geometry. Journal of Chemical Physics, 2012, 137, 194110.	1.2	8
83	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
84	Local Disorder in Lithium Imide from Density Functional Simulation and NMR Spectroscopy. Journal of Physical Chemistry C, 2012, 116, 18577-18583.	1.5	6
85	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
86	Hydrogen bond networks: Structure and dynamics via firstâ€principles spectroscopy. Physica Status Solidi (B): Basic Research, 2012, 249, 368-375.	0.7	10
87	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
88	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
89	Dinitrogen complexation with main group radicals. Chemical Science, 2011, 2, 473-479.	3.7	15
90	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

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91	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
92	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
93	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
94	Self-Assembly of Dendronized Perylene Bisimides into Complex Helical Columns. Journal of the American Chemical Society, 2011, 133, 12197-12219.	6.6	120
95	Empty Helical Nanochannels with Adjustable Order from Lowâ€Symmetry Macrocycles. Angewandte Chemie - International Edition, 2011, 50, 3030-3033.	7.2	79
96	Specific quantum mechanical/molecular mechanical capping-potentials for biomolecular functional groups. Journal of Chemical Physics, 2011, 135, 214107.	1.2	18
97	Local Disorder in Hydrogen Storage Compounds: The Case of Lithium Amide/Imide. ChemPhysChem, 2010, 11, 2353-2360.	1.0	22
98	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
99	Molecular Mechanisms of Additive Fortification in Model Epoxy Resins: A Solid State NMR Study. Macromolecules, 2010, 43, 7200-7211.	2.2	9
100	Possibility of Coherent Delocalized Nuclear Quantum States of Protons in Li₂NH. Journal of Physical Chemistry Letters, 2010, 1, 3214-3218.	2.1	7
101	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
102	Polyhedral Phenylacetylenes: The Interplay of Aromaticity and Antiaromaticity in Convex Graphyne Substructures. Symmetry, 2009, 1, 226-239.	1.1	8
103	Solid-state NMR and computational studies of tetratolyl urea calix[4]arene inclusion compounds. Physical Chemistry Chemical Physics, 2009, 11, 9241.	1.3	15
104	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
105	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
106	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
107	Electronic Response Properties of Carbon Nanotubes in Magnetic Fields. ACS Nano, 2008, 2, 661-668.	7.3	57
108	Beyond Isotropic Tumbling Models: Nuclear Spin Relaxation in Liquids from First Principles. ChemPhysChem, 2008, 9, 2313-2316.	1.0	28

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109	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
110	Proton momentum distribution in water: an open path integral molecular dynamics study. Journal of Chemical Physics, 2007, 126, 234504.	1.2	66
111	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
112	Selectivity of guestâ€“host interactions in self-assembled hydrogen-bonded nanostructures observed by NMR. Physical Chemistry Chemical Physics, 2007, 9, 4545.	1.3	28
113	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
114	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
115	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
116	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
117	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
118	From Armchair to Zigzag Peripheries in Nanographenes. Journal of the American Chemical Society, 2006, 128, 9526-9534.	6.6	153
119	Current Densities and Nucleus-Independent Chemical Shift Maps from Reciprocal-Space Density Functional Perturbation Theory Calculations. ChemPhysChem, 2006, 7, 164-175.	1.0	89
120	Vibrational Frequencies of Water Adsorbed on (111) and (221) Nickel Surfaces from First Principle Calculations. ChemPhysChem, 2006, 7, 1215-1219.	1.0	27
121	First Principles and Experimental 1H NMR Signatures of Solvated Ions: The Case of HCl(aq). ChemPhysChem, 2006, 7, 2578-2584.	1.0	43
122	Performance of optimized atom-centered potentials for weakly bonded systems using density functional theory. Physical Review B, 2005, 71, .	1.1	107
123	Crystalline diamond polymorphs analyzed with first-principles13C NMR chemical shift calculations. International Journal of Quantum Chemistry, 2005, 101, 849-853.	1.0	3
124	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
125	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
126	Variational optimization of effective atom centered potentials for molecular properties. Journal of Chemical Physics, 2005, 122, 014113.	1.2	110

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127	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
128	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
129	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
130	Visualizing Degrees of Aromaticity for Different Barbaralane Systems. Journal of Physical Chemistry A, 2004, 108, 11728-11732.	1.1	21
131	Nuclear Magnetic Resonance Chemical Shifts from Hybrid DFT QM/MM Calculations. Journal of Physical Chemistry B, 2004, 108, 2807-2815.	1.2	58
132	Optimization of Effective Atom Centered Potentials for London Dispersion Forces in Density Functional Theory. Physical Review Letters, 2004, 93, 153004.	2.9	489
133	Low temperature annealing in tetrahedral amorphous carbon thin films observed by13CNMR spectroscopy. Physical Review B, 2003, 67, .	1.1	47
134	NMR chemical shifts in proton conducting crystals from first principles. Computational and Theoretical Chemistry, 2003, 625, 283-288.	1.5	28
135	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
136	AB-INITIO CALCULATIONS OF NMR PARAMETERS IN CONDENSED PHASES. Modern Physics Letters B, 2003, 17, 1301-1319.	1.0	31
137	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
138	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
139	Ab-initio Study of NMR Chemical Shifts of Water Under Normal and Supercritical Conditions. ChemPhysChem, 2002, 3, 675.	1.0	65
140	NMR chemical shifts in periodic systems from first principles. Computer Physics Communications, 2002, 147, 707-710.	3.0	45
141	Is NMR the tool to characterize the structure of C20 isomers?. Chemical Physics Letters, 2002, 366, 134-140.	1.2	22
142	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
143	A New ab-Initio Approach for NMR Chemical Shifts in Periodic Systems. Journal of Physical Chemistry A, 2001, 105, 1951-1958.	1.1	207
144	Accurate Total Energies without Self-Consistency. Physical Review Letters, 2001, 87, 226401.	2.9	24

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145	Generalized variational density functional perturbation theory. Journal of Chemical Physics, 2000, 113, 7102-7109.	1.2	183
146	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