Riccardo Spezia

List of Publications by Year
in descending order

129 papers	3,239 citations	159525 30 h-index	206029 48 g-index
154 all docs	154 docs citations	154 times ranked	2867 citing authors

#	Article	IF	Citations
1	Thermochemical and conformational studies of Ni(II) and Zn(II) ternary complexes of alternative metal binding peptides with nitrilotriacetic acid. International Journal of Mass Spectrometry, 2022, 473, 116792.	0.7	3
2	How Symmetry Influences the Dissociation of Protonated Cyclic Peptides. Symmetry, 2022, 14, 679.	1.1	4
3	Speciation and thermodynamic properties of La(III)-Cl complexes in hydrothermal fluids: A combined molecular dynamics and in situ X-ray absorption spectroscopy study. Geochimica Et Cosmochimica Acta, 2022, 330, 27-46.	1.6	5
4	Efficient and Accurate Description of Dielsâ€Alder Reactions Using Density Functional Theory**. ChemPhysChem, 2022, 23, .	1.0	6
5	In Silico Tandem Mass Spectrometer: an Analytical and Fundamental Tool. Chemistry Methods, 2021, 1, 123-130.	1.8	5
6	Formation of Co(II), Ni(II), Zn(II) complexes of alternative metal binding heptapeptides and nitrilotriacetic acid: Discovering new potential affinity tags. International Journal of Mass Spectrometry, 2021, 463, 116554.	0.7	7
7	Structure and collision-induced dissociation of the protonated cyclo His-Phe dipeptide: mechanistic studies and stereochemical effects. European Physical Journal D, 2021, 75, 1.	0.6	7
8	Stereospecific collision-induced dissociation and vibrational spectroscopy of protonated cyclo (Tyr-Pro). International Journal of Mass Spectrometry, 2021, 465, 116590.	0.7	7
9	Determination of kinetic properties in unimolecular dissociation of complex systems from graph theory based analysis of an ensemble of reactive trajectories. Journal of Chemical Physics, 2021, 155, 124103.	1.2	7
10	Unimolecular Fragmentation Properties of Thermometer Ions from Chemical Dynamics Simulations. Journal of the American Society for Mass Spectrometry, 2021, 32, 169-179.	1.2	5
11	Collisional dynamics simulations revealing fragmentation properties of Zn(<scp>ii</scp>)-bound poly-peptide. Physical Chemistry Chemical Physics, 2020, 22, 14551-14559.	1.3	5
12	Exploring reactivity and product formation in N(4S) collisions with pristine and defected graphene with direct dynamics simulations. Journal of Chemical Physics, 2020, 153, 184702.	1.2	13
13	Computer simulation of collision induced dissociation and isolobal analogy: The case of biotin and its analogs. International Journal of Mass Spectrometry, 2020, 457, 116417.	0.7	0
14	Role of Chemical Dynamics Simulations in Mass Spectrometry Studies of Collision-Induced Dissociation and Collisions of Biological Ions with Organic Surfaces. Journal of the American Society for Mass Spectrometry, 2020, 31, 2-24.	1.2	30
15	Infraredâ€Assisted Synthesis of Prebiotic Glycine. ChemPhysChem, 2020, 21, 503-509.	1.0	3
16	Solvation effects drive the selectivity in Dielsâ€“Alder reaction under hyperbaric conditions. Chemical Communications, 2020, 56, 6632-6635.	2.2	12
17	On the formation of propylene oxide from propylene in space: gas-phase reactions. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	3
18	Singlet oxygen from cation driven superoxide disproportionation and consequences for aprotic metalâ€“O₂ batteries. Energy and Environmental Science, 2019, 12, 2559-2568.	15.6	122

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19	Fragmentation Spectra Prediction and DNA Adducts Structural Determination. Journal of the American Society for Mass Spectrometry, 2019, 30, 2771-2784.	1.2	10
20	On the Use of Quantum Thermal Bath in Unimolecular Fragmentation Simulation. Journal of Physical Chemistry A, 2019, 123, 8542-8551.	1.1	5
21	Response to â€œComment on â€˜On the development of polarizable and Lennard-Jones force fields to study hydration structure and dynamics of actinide(III) ions based on effective ionic radiiâ€™â€•[J. Chem. Phys. 150, 097101 (2019)]. Journal of Chemical Physics, 2019, 150, 097102.	1.2	0
22	<scp>l</scp>-Cysteine Modified by S-Sulfation: Consequence on Fragmentation Processes Elucidated by Tandem Mass Spectrometry and Chemical Dynamics Simulations. Journal of Physical Chemistry A, 2019, 123, 3685-3696.	1.1	20
23	The formation of urea in space. II. MP2 versus PM6 dynamics in determining bimolecular reaction products. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	21
24	Unimolecular Fragmentation of Deprotonated Diproline [Pro₂-H]^{â^'} Studied by Chemical Dynamics Simulations and IRMPD Spectroscopy. Journal of Physical Chemistry A, 2018, 122, 2612-2625.	1.1	18
25	Chemical dynamics simulations of CID of peptide ions: comparisons between TIK(H⁺)₂and TLK(H⁺)₂fragmentation dynamics, and with thermal simulations. Physical Chemistry Chemical Physics, 2018, 20, 3614-3629.	1.3	18
26	Degradation of LiTfO/TEGME and LiTfO/DME Electrolytes in Li-O₂Batteries. Journal of the Electrochemical Society, 2018, 165, A118-A125.	1.3	33
27	Gas Phase Synthesis of Protonated Glycine by Chemical Dynamics Simulations. Journal of Physical Chemistry A, 2018, 122, 869-877.	1.1	19
28	Graph theory for automatic structural recognition in molecular dynamics simulations. Journal of Chemical Physics, 2018, 149, 184102.	1.2	15
29	TileViz : Tile visualization for direct dynamics applied to astrochemical reactions.. IS&T International Symposium on Electronic Imaging, 2018, 2018, 286-1-286-7.	0.3	1
30	Ionâ€“Molecule Reactions as a Possible Synthetic Route for the Formation of Prebiotic Molecules in Space. , 2018, , 277-292.		2
31	Threshold for shattering fragmentation in collision-induced dissociation of the doubly protonated tripeptide TIK(H⁺)₂. Physical Chemistry Chemical Physics, 2018, 20, 19744-19749.	1.3	13
32	The formation of urea in space. Astronomy and Astrophysics, 2018, 610, A26.	2.1	16
33	Excited state characterization of carbonyl containing carotenoids: a comparison between single and multireference descriptions. Physical Chemistry Chemical Physics, 2017, 19, 17156-17166.	1.3	15
34	Characterization of Protonated Model Disaccharides from Tandem Mass Spectrometry and Chemical Dynamics Simulations. ChemPhysChem, 2017, 18, 2812-2823.	1.0	22
35	Theoretical and computational studies of non-equilibrium and non-statistical dynamics in the gas phase, in the condensed phase and at interfaces. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20170035.	1.6	18
36	Fermi resonance in CO2: Mode assignment and quantum nuclear effects from first principles molecular dynamics. Journal of Chemical Physics, 2017, 146, 134102.	1.2	19

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37	How Does Ce^{III} Nitrate Dissolve in a Protic Ionic Liquid? A Combined Molecular Dynamics and EXAFS Study. Chemistry - A European Journal, 2017, 23, 8424-8433.	1.7	19
38	Gas-phase reactivity of [Ca(formamide)] ²⁺ complex: an example of different dynamical behaviours. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20160196.	1.6	6
39	Solvation Properties of the Actinide Ion Th(IV) in DMSO and DMSO:Water Mixtures through Polarizable Molecular Dynamics. Inorganic Chemistry, 2017, 56, 11929-11937.	1.9	3
40	On the development of polarizable and Lennard-Jones force fields to study hydration structure and dynamics of actinide(III) ions based on effective ionic radii. Journal of Chemical Physics, 2017, 147, 161707.	1.2	30
41	Structural and energetic properties of La3+ in water/DMSO mixtures. Journal of Molecular Structure, 2017, 1148, 381-387.	1.8	2
42	Lutetium(iii) aqua ion: On the dynamical structure of the heaviest lanthanoid hydration complex. Journal of Chemical Physics, 2016, 144, 204505.	1.2	15
43	On the gas phase fragmentation of protonated uracil: a statistical perspective. Physical Chemistry Chemical Physics, 2016, 18, 14980-14990.	1.3	34
44	Unimolecular dissociation of peptides: statistical vs. non-statistical fragmentation mechanisms and time scales. Faraday Discussions, 2016, 195, 599-618.	1.6	27
45	Model Simulations of the Thermal Dissociation of the TIK(H+)2 Tripeptide: Mechanisms and Kinetic Parameters. Journal of Physical Chemistry A, 2016, 120, 8211-8227.	1.1	34
46	Gas phase fragmentation mechanisms of protonated testosterone as revealed by chemical dynamics simulations. International Journal of Mass Spectrometry, 2016, 407, 40-50.	0.7	13
47	Gas phase vibrational spectroscopy of the protonated water pentamer: the role of isomers and nuclear quantum effects. Physical Chemistry Chemical Physics, 2016, 18, 26743-26754.	1.3	53
48	1,2â€Dimethoxyethane Degradation Thermodynamics in Liâ"O₂ Redox Environments. Chemistry - A European Journal, 2016, 22, 17188-17203.	1.7	23
49	SYNTHESIS OF FORMAMIDE AND RELATED ORGANIC SPECIES IN THE INTERSTELLAR MEDIUM VIA CHEMICAL DYNAMICS SIMULATIONS. Astrophysical Journal, 2016, 826, 107.	1.6	24
50	Frontispiece: 1,2â€Dimethoxyethane Degradation Thermodynamics in Liâ"O₂ Redox Environments. Chemistry - A European Journal, 2016, 22, .	1.7	0
51	Post-Transition State Dynamics in Gas Phase Reactivity: Importance of Bifurcations and Rotational Activation. Journal of Chemical Theory and Computation, 2016, 12, 974-982.	2.3	22
52	Structure, Stability, and Electronic Properties of Dimethyl Sulfoxide and Dimethyl Formammide Clusters Containing Th⁴⁺. Journal of Physical Chemistry A, 2016, 120, 4778-4788.	1.1	3
53	Elucidating collision induced dissociation products and reaction mechanisms of protonated uracil by coupling chemical dynamics simulations with tandem mass spectrometry experiments. Journal of Mass Spectrometry, 2015, 50, 1340-1351.	0.7	31
54	Echinenone vibrational properties: From solvents to the orange carotenoid protein. Biochimica Et Biophysica Acta - Bioenergetics, 2015, 1847, 1044-1054.	0.5	48

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55	Collision-induced dissociation mechanisms of protonated penta- and octa-glycine as revealed by chemical dynamics simulations. International Journal of Mass Spectrometry, 2015, 392, 125-138.	0.7	27
56	Stalking Higher Energy Conformers on the Potential Energy Surface of Charged Species. Journal of Chemical Theory and Computation, 2015, 11, 871-883.	2.3	16
57	Assignment of IR bands of isolated and protein-bound Peridinin in its fundamental and triplet state by static FTIR, time-resolved step-scan FTIR and DFT calculations. Journal of Molecular Structure, 2015, 1090, 58-64.	1.8	9
58	Solvent Structure around Lanthanoid(III) Ions in Liquid DMSO As Revealed by Polarizable Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2015, 119, 13347-13357.	1.2	5
59	Collision-induced dissociation pathways of protonated Gly2NH2 and Gly3NH2 in the short time-scale limit by chemical dynamics and ion spectroscopy. International Journal of Mass Spectrometry, 2015, 388, 40-52.	0.7	34
60	XAS examination of glutathioneâ€“cobalt complexes in solution. Journal of Inorganic Biochemistry, 2015, 142, 126-131.	1.5	6
61	The Unique Photophysical Properties of the Peridinin-Chlorophyll-a-Protein. Current Protein and Peptide Science, 2014, 15, 332-350.	0.7	35
62	Structural, Energetic, and Electronic Properties of La(III)â€“Dimethyl Sulfoxide Clusters. Journal of Physical Chemistry A, 2014, 118, 11602-11611.	1.1	4
63	UO₂²⁺ Uptake by Proteins: Understanding the Binding Features of the Super Uranyl Binding Protein and Design of a Protein with Higher Affinity. Journal of the American Chemical Society, 2014, 136, 17484-17494.	6.6	74
64	Theoretical Methods for Vibrational Spectroscopy and Collision Induced Dissociation in the Gas Phase. Topics in Current Chemistry, 2014, 364, 99-151.	4.0	22
65	Galactose-6-Sulfate collision induced dissociation using QM+MM chemical dynamics simulations and ESI-MS/MS experiments. International Journal of Mass Spectrometry, 2014, 358, 25-35.	0.7	31
66	Hydration properties of Cm(iii) and Th(iv) combining coordination free energy profiles with electronic structure analysis. Physical Chemistry Chemical Physics, 2014, 16, 5824.	1.3	21
67	Uranylâ€“Peroxide Nanocapsules in Aqueous Solution: Force Field Development and First Applications. Journal of Physical Chemistry C, 2014, 118, 24730-24740.	1.5	22
68	A RRKM study and a DFT assessment on gas-phase fragmentation of formamideâ€“M2+ (M = Ca, Sr). Physical Chemistry Chemical Physics, 2014, 16, 14813.	1.3	7
69	Hydration properties of lanthanoid(iii) carbonate complexes in liquid water determined by polarizable molecular dynamics simulations. Physical Chemistry Chemical Physics, 2014, 16, 3693.	1.3	15
70	Unimolecular Fragmentation Induced By Low-Energy Collision: Statistically or Dynamically Driven?. Journal of Physical Chemistry A, 2014, 118, 10882-10893.	1.1	26
71	Perfluoroalkyl-Fluorophosphate Anions for High Voltage Electrolytes in Lithium Cells: DFT Study. Journal of Physical Chemistry C, 2014, 118, 24221-24230.	1.5	13
72	Developing polarizable potential for molecular dynamics of Cm(III)-carbonate complexes in liquid water. Journal of Molecular Modeling, 2014, 20, 2398.	0.8	3

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73	Fermi Resonance as a Tool for Probing Peridinin Environment. Journal of Physical Chemistry B, 2014, 118, 5873-5881.	1.2	24
74	Conical intersection structure and dynamics for a model protonated schiff base photoisomerization in solution. International Journal of Quantum Chemistry, 2013, 113, 296-305.	1.0	7
75	Easy eco-friendly phenonium ion production from phenethyl alcohols in dimethyl carbonate. Tetrahedron Letters, 2013, 54, 5004-5006.	0.7	7
76	K-edge XANES investigation of octakis(DMSO)lanthanoid(iii) complexes in DMSO solution and solid iodides. Physical Chemistry Chemical Physics, 2013, 15, 8684.	1.3	15
77	Hydration Properties and Ionic Radii of Actinide(III) Ions in Aqueous Solution. Inorganic Chemistry, 2013, 52, 10318-10324.	1.9	80
78	Gas-phase collision induced dissociation mechanisms of peptides: Theoretical and experimental study of N-formylalanylamide fragmentation. International Journal of Mass Spectrometry, 2013, 335, 33-44.	0.7	30
79	Reactivity of lanthanoid mono-cations with ammonia: A combined inductively coupled plasma mass spectrometry and computational investigation. International Journal of Mass Spectrometry, 2013, 334, 27-37.	0.7	12
80	p of silicic acid in presence of La³⁺using single sweep method coupled to DFT-based molecular dynamics. Molecular Physics, 2013, 111, 3478-3485.	0.8	1
81	Charge localization in multiply charged clusters and their electrical properties: Some insights into electrospray droplets. Journal of Chemical Physics, 2012, 136, 184503.	1.2	9
82	Structure and stability of charged clusters. Journal of Physics Condensed Matter, 2012, 24, 284130.	0.7	8
83	Unravelling the Hydration Structure of ThX₄ (X = Br, Cl) Water Solutions by Molecular Dynamics Simulations and X-ray Absorption Spectroscopy. Journal of Physical Chemistry B, 2012, 116, 6465-6475.	1.2	28
84	Collision induced dissociation of doubly-charged ions: Coulomb explosion vs. neutral loss in [Ca(urea)]2+ gas phase unimolecular reactivity via chemical dynamics simulations. Physical Chemistry Chemical Physics, 2012, 14, 11724.	1.3	25
85	Electronic structure and bonding of lanthanoid(iii) carbonates. Physical Chemistry Chemical Physics, 2012, 14, 14822.	1.3	38
86	Varying the charge of small cations in liquid water: Structural, transport, and thermodynamical properties. Journal of Chemical Physics, 2012, 137, 164501.	1.2	9
87	Hydration of Lanthanoids(III) and Actinoids(III): An Experimental/Theoretical Saga. Chemistry - A European Journal, 2012, 18, 11162-11178.	1.7	114
88	A non-comparative assessment of tolerability and efficacy of duloxetine in the treatment of depressed patients with Parkinson's disease. Expert Opinion on Pharmacotherapy, 2012, 13, 2269-2280.	0.9	25
89	Lanthanoids(III) and actinoids(III) in water: Diffusion coefficients and hydration enthalpies from polarizable molecular dynamics simulations. Pure and Applied Chemistry, 2012, 85, 237-246.	0.9	33
90	Environmental effects on vibrational properties of carotenoids: experiments and calculations on peridinin. Physical Chemistry Chemical Physics, 2011, 13, 20954.	1.3	45

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91	Dynamical Friction Effects on the Photoisomerization of a Model Protonated Schiff Base in Solution. Journal of Physical Chemistry A, 2011, 115, 3720-3735.	1.1	43
92	Stability and Instability of the Isoelectronic UO22+and PaO2+Actinyl Oxo-Cations in Aqueous Solution from Density Functional Theory Based Molecular Dynamics. Journal of Physical Chemistry B, 2011, 115, 3560-3570.	1.2	22
93	Revised Ionic Radii of Lanthanoid(III) Ions in Aqueous Solution. Inorganic Chemistry, 2011, 50, 4572-4579.	1.9	212
94	Collision induced dissociation of protonated urea with N2: Effects of rotational energy on reactivity and energy transfer via chemical dynamics simulations. International Journal of Mass Spectrometry, 2011, 308, 289-298.	0.7	26
95	Polarizable interaction potential for molecular dynamics simulations of actinoids(III) in liquid water. Journal of Chemical Physics, 2011, 135, 044503.	1.2	28
96	Cu2+ binding chalcogenâ€“chalcogen bridges: A problematic case for DFT. Computational and Theoretical Chemistry, 2010, 954, 7-15.	1.5	12
97	Temperature influence on lanthanoids (III) hydration from molecular dynamics simulations. Chemical Physics Letters, 2010, 498, 90-96.	1.2	12
98	Density functional theory based molecular dynamics study of hydration and electronic properties of aqueous La3+. Journal of Chemical Physics, 2010, 133, 044509.	1.2	36
99	Hydration of Lanthanide Chloride Salts: A Quantum Chemical and Classical Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2010, 114, 15590-15597.	1.2	60
100	An Ab Initio Molecular Dynamics Study on the Hydrolysis of the Po(IV) Aquaion in Water. Journal of Physical Chemistry B, 2010, 114, 12866-12874.	1.2	17
101	What first principles molecular dynamics can tell us about EXAFS spectroscopy of radioactive heavy metal cations in water. Radiochimica Acta, 2009, 97, 339-346.	0.5	22
102	Building a polarizable pair interaction potential for lanthanoids(III) in liquid water: A molecular dynamics study of structure and dynamics of the whole series. Journal of Chemical Physics, 2009, 130, 104501.	1.2	88
103	Protonated Urea Collision-Induced Dissociation. Comparison of Experiments and Chemical Dynamics Simulations. Journal of Physical Chemistry A, 2009, 113, 13853-13862.	1.1	60
104	Mn2+-, Fe2+-, Co2+-, Ni2+-, Cu2+-, and Zn2+-Binding Chalcogenâ^'Chalcogen Bridges: A Compared MP2 and B3LYP Study. Journal of Physical Chemistry A, 2009, 113, 7878-7887.	1.1	20
105	Molecular dynamics to rationalize EXAFS experiments: A dynamical model explaining hydration behaviour across the lanthanoid(III) series. Journal of Physics: Conference Series, 2009, 190, 012056.	0.3	11
106	A Dynamic Model to Explain Hydration Behaviour along the Lanthanide Series. ChemPhysChem, 2008, 9, 693-696.	1.0	86
107	Solvation of Co(III)-Cysteinato Complexes in Water: A DFT-based Molecular Dynamics Study. Journal of Physical Chemistry B, 2008, 112, 6490-6499.	1.2	20
108	Time-resolved step scan FTIR spectroscopy and DFT investigation on triplet formation in peridininâ€“chlorophyll-aâ€“protein from Amphidinium carterae at low temperature. Spectroscopy, 2008, 22, 235-250.	0.8	20

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109	Pair interaction potentials with explicit polarization for molecular dynamics simulations of La3+ in bulk water. Journal of Chemical Physics, 2007, 127, 034503.	1.2	67
110	A combined spectroscopic and theoretical approach to investigate structural properties of Co(ii)/Co(iii) tris-cysteinato complexes in aqueous medium. New Journal of Chemistry, 2007, 31, 1789.	1.4	14
111	Structures and fragmentations of Cobalt(II)â€“cysteine complexes in the gas phase. Journal of Mass Spectrometry, 2007, 42, 517-526.	0.7	24
112	Temperature dependence of hydrated La3+ properties in liquid water, a molecular dynamics simulations study. Chemical Physics Letters, 2007, 448, 41-45.	1.2	23
113	A Coupled Car-Parrinello Molecular Dynamics and EXAFS Data Analysis Investigation of Aqueous Co2+. Journal of Physical Chemistry A, 2006, 110, 13081-13088.	1.1	46
114	Toward a DFT-based molecular dynamics description of Co(ii) binding in sulfur-rich peptides. Physical Chemistry Chemical Physics, 2006, 8, 2040.	1.3	27
115	Co2+Binding Cysteine and Selenocysteine:Â A DFT Study. Journal of Physical Chemistry A, 2006, 110, 9727-9735.	1.1	41
116	An interdisciplinary approach toÂinvestigate theÂimpact ofÂcobalt inÂaÂhuman keratinocyte cell line. Biochimie, 2006, 88, 1619-1629.	1.3	18
117	Conical intersections in solution: non-equilibrium versus equilibrium solvation. Molecular Physics, 2006, 104, 903-914.	0.8	40
118	Solvation and Photochemical Funnels. , 2006, , 143-153.		1
119	Molecular dynamics simulations of the temperature and density dependence of the absorption spectra of hydrated electron and solvated silver atom in water. Chemical Physics Letters, 2005, 409, 219-223.	1.2	14
120	Molecular dynamics simulations of the Ag+ or Na+ cation with an excess electron in bulk water. Journal of Chemical Physics, 2004, 120, 5261-5268.	1.2	30
121	THEORETICAL STUDY OF NEUTRAL DIPOLAR ATOM IN WATER: STRUCTURE, SPECTROSCOPY AND FORMATION OF AN EXCITONIC STATE. Modern Physics Letters B, 2004, 18, 1327-1345.	1.0	3
122	Reactivity of an Excess Electron with Monovalent Cations in Bulk Water by Mixed Quantum Classical Molecular Dynamics Simulations. Molecular Simulation, 2004, 30, 749-754.	0.9	3
123	Conformational fluctuations and electronic properties in myoglobin. Journal of Computational Chemistry, 2004, 25, 974-984.	1.5	35
124	A DFT Study of the Low-Lying Singlet Excited States of the All-Trans Peridinin in vacuo. Journal of Physical Chemistry A, 2004, 108, 6763-6770.	1.1	21
125	The Effect of Protein Conformational Flexibility on the Electronic Properties of a Chromophore. Biophysical Journal, 2003, 84, 2805-2813.	0.2	36
126	Molecular Dynamics Simulations of a Silver Atom in Water: Evidence for a Dipolar Excitonic State. Physical Review Letters, 2003, 91, 208304.	2.9	28

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127	A first principles polarizable water model for molecular simulations: application to a water dimer. Journal of Molecular Liquids, 2002, 101, 181-198.	2.3	9
128	Extension of the perturbed matrix method: application to a water molecule. Chemical Physics Letters, 2002, 365, 450-456.	1.2	51
129	A first-principles method to model perturbed electronic wavefunctions: the effect of an external homogeneous electric field. Chemical Physics Letters, 2001, 344, 374-380.	1.2	120