Rajendra R Zope

List of Publications by Year
in descending order

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81 papers	1,616 citations	257357 24 h-index	360920 35 g-index
81 all docs	81 docs citations	81 times ranked	1190 citing authors

#	Article	IF	Citations
1	Study of self-interaction-errors in barrier heights using locally scaled and Perdewâ€“Zunger self-interaction methods. Journal of Chemical Physics, 2022, 156, 014306.	1.2	12
2	Study of Self-Interaction Errors in Density Functional Calculations of Magnetic Exchange Coupling Constants Using Three Self-Interaction Correction Methods. Journal of Physical Chemistry A, 2022, 126, 1923-1935.	1.1	6
3	Local self-interaction correction method with a simple scaling factor. Physical Chemistry Chemical Physics, 2021, 23, 2406-2418.	1.3	14
4	Density-related properties from self-interaction corrected density functional theory calculations. Journal of Chemical Physics, 2021, 154, 024102.	1.2	8
5	Implementation of Perdewâ€“Zunger self-interaction correction in real space using Fermiâ€“LÃ¶wdin orbitals. Journal of Chemical Physics, 2021, 154, 084112.	1.2	7
6	Static dipole polarizabilities of polyacenes using self-interaction-corrected density functional approximations. Journal of Chemical Physics, 2021, 154, 114305.	1.2	12
7	Exploring and enhancing the accuracy of interior-scaled Perdewâ€“Zunger self-interaction correction. Journal of Chemical Physics, 2021, 154, 094105.	1.2	12
8	Fermi-LÃ¶wdin-orbital self-interaction correction using the optimized-effective-potential method within the Krieger-Li-Iafrate approximation. Physical Review A, 2021, 103, .	1.0	14
9	Magnetic structure, excitations and short-range order in honeycomb Na2Ni2TeO6. Journal of Physics Condensed Matter, 2021, 33, 375803.	0.7	3
10	Self-interaction-corrected Kohnâ€“Sham effective potentials using the density-consistent effective potential method. Journal of Chemical Physics, 2021, 155, 064109.	1.2	8
11	How well do self-interaction corrections repair the overestimation of static polarizabilities in density functional calculations?. Physical Chemistry Chemical Physics, 2021, 23, 18678-18685.	1.3	14
12	Importance of self-interaction-error removal in density functional calculations on water cluster anions. Physical Chemistry Chemical Physics, 2020, 22, 3789-3799.	1.3	32
13	Assessing the effect of regularization on the molecular properties predicted by SCAN and self-interaction corrected SCAN meta-GGA. Physical Chemistry Chemical Physics, 2020, 22, 18060-18070.	1.3	6
14	Study of self-interaction errors in density functional predictions of dipole polarizabilities and ionization energies of water clusters using Perdewâ€“Zunger and locally scaled self-interaction corrected methods. Journal of Chemical Physics, 2020, 153, 164304.	1.2	21
15	Self-interaction error overbinds water clusters but cancels in structural energy differences. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 11283-11288.	3.3	57
16	Improvements in the orbitalwise scaling down of Perdewâ€“Zunger self-interaction correction in many-electron regions. Journal of Chemical Physics, 2020, 152, 174112.	1.2	23
17	A step in the direction of resolving the paradox of Perdewâ€“Zunger self-interaction correction. II. Gauge consistency of the energy density at three levels of approximation. Journal of Chemical Physics, 2020, 152, 214109.	1.2	23
18	Self-interaction-free electric dipole polarizabilities for atoms and their ions using the Fermi-LÃ¶wdin self-interaction correction. Physical Review A, 2019, 100, .	1.0	27

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19	The effect of self-interaction error on electrostatic dipoles calculated using density functional theory. Journal of Chemical Physics, 2019, 151, 174106.	1.2	29
20	Stretched or noded orbital densities and self-interaction correction in density functional theory. Journal of Chemical Physics, 2019, 150, 174102.	1.2	46
21	Fermi-LÃ¶wdin orbital self-interaction correction using the strongly constrained and appropriately normed meta-GGA functional. Journal of Chemical Physics, 2019, 151, 154105.	1.2	38
22	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. Journal of Chemical Physics, 2019, 151, 214108.	1.2	56
23	Analytic atomic gradients in the fermiâ€‰LÃ¶wdin orbital selfâ€‰interaction correction. Journal of Computational Chemistry, 2019, 40, 820-825.	1.5	16
24	Shrinking Self-Interaction Errors with the Fermiâ€“LÃ¶wdin Orbital Self-Interaction-Corrected Density Functional Approximation. Journal of Physical Chemistry A, 2018, 122, 9307-9315.	1.1	30
25	Electronic structure calculation of vanadiumâ€and scandiumâ€based endohedral fullerenes VSc₂N@C_{2n} (2n = 70, 76, 78, 80). International Journal of Quantum Chemistry, 2018, 118, e25785.	1.0	2
26	Fermi-LÃ¶wdin orbital self-interaction correction to magnetic exchange couplings. Journal of Chemical Physics, 2018, 149, 164101.	1.2	33
27	A DFT analysis of the ground and charge-transfer excited states of Sc₃N@I_hâ€“C₈₀ fullerene coupled with metal-free and zinc-phthalocyanine. Physical Chemistry Chemical Physics, 2018, 20, 25841-25848.	1.3	10
28	On the Question of the Total Energy in the Fermiâ€“LÃ¶wdin Orbital Self-Interaction Correction Method. Journal of Chemical Theory and Computation, 2018, 14, 4122-4128.	2.3	22
29	Electronic and Structural Study of Zn_xS_x [x = 12, 16, 24, 28, 36, 48, 96, and 108] Cage Structures. Journal of Physical Chemistry A, 2017, 121, 3486-3493.	1.1	6
30	Donor-fullerene dyads for energy cascade organic solar cells. Inorganica Chimica Acta, 2017, 468, 192-202.	1.2	10
31	Diels-Alder addition to H2O@C60 an electronic and structural study. Chemical Physics Letters, 2017, 685, 198-204.	1.2	4
32	Density functional study of the electronic structure of dye-functionalized fullerenes and their model donor-acceptor complexes containing P3HT. Journal of Chemical Physics, 2016, 144, 144304.	1.2	7
33	Excited Electronic States of Porphyrin-Based Assemblies Using Density Functional Theory. , 2016, , 233-289.		1
34	Electronic and Optical Properties of VSc₂N@C₆₈ Fullerene. Journal of Physical Chemistry C, 2016, 120, 27813-27819.	1.5	7
35	Electronic and Structural Properties of C₆₀ and Sc₃N@C₈₀ Supported on Graphene Nanoflakes. Journal of Physical Chemistry C, 2016, 120, 26083-26092.	1.5	11
36	Al₁₂Cu Superatom as Stable Building Block of Ionic Salts. Journal of Physical Chemistry C, 2015, 119, 5129-5137.	1.5	25

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37	The electronic structure and charge transfer excited states of the endohedral trimetallic nitride C₈₀ (I_h) fullerenesâ€“Zn-tetraphenyl porphyrin dyads. Physical Chemistry Chemical Physics, 2015, 17, 5832-5839.	1.3	17
38	Site specific atomic polarizabilities in endohedral fullerenes and carbon onions. Journal of Chemical Physics, 2015, 143, 084306.	1.2	11
39	Crystalline Alloys of Organic Donors and Acceptors Based on TIPS-Pentacene. Journal of Physical Chemistry C, 2015, 119, 20823-20832.	1.5	14
40	The effect of structural changes on charge transfer states in a light-harvesting carotenoid-diaryl-porphyrin-C60 molecular triad. Journal of Chemical Physics, 2014, 140, 204309.	1.2	8
41	Geometry and electronic structure of neutral and charged B21 clusters. Chemical Physics Letters, 2013, 557, 15-18.	1.2	13
42	Smooth scaling of valence electronic properties in fullerenes: From one carbon atom, to C<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>60</mml:mn></mml:msub></mml:math>, to graphene. Physical Review A, 2013, 87, .	1.0	5
43	Low-lying planar isomers of neutral and charged B₂₂clusters. Journal of Physics B: Atomic, Molecular and Optical Physics, 2012, 45, 225101.	0.6	17
44	Charge transfer excited state energies by perturbative delta self consistent field method. Journal of Chemical Physics, 2012, 137, 084316.	1.2	35
45	Charge transfer excitations in cofacial fullerene-porphyrin complexes. Journal of Chemical Physics, 2012, 137, 084317.	1.2	26
46	Calcium coated B80 fullerene: A study on various coating configurations of B80. Chemical Physics Letters, 2011, 514, 66-69.	1.2	11
47	Snub boron nanostructures: Chiral fullerenes, nanotubes and planar sheet. Chemical Physics Letters, 2011, 501, 193-196.	1.2	69
48	Optical excitation energies, Stokes shift, and spin-splitting of C24H72Si14. Journal of Chemical Physics, 2010, 133, 034301.	1.2	14
49	Boron fullerenes: From<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>B</mml:mtext><mml:mrow><mml:mn>80</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> hole doped boron sheets. Physical Review B, 2009, 79, .	1.1	64
50	Dipole polarizability of isovalent carbon and boron cages and fullerenes. Physical Review B, 2009, 80, .	1.1	16
51	The Î±-boron cages with four-member rings. Europhysics Letters, 2009, 85, 68005.	0.7	28
52	Comparative study of unscreened and screened molecular static linear polarizability in the Hartreeâ€“Fock, hybridâ€density functional, and density functional models. International Journal of Quantum Chemistry, 2008, 108, 307-317.	1.0	14
53	[illegible] fullerenes from<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:math>to<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>2160</mml:mn></mml:msub></mml:math>characterized by [illegible] 2008, 77, .	1.1	58
54	Vibrational stability and electronic structure of a<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>B</mml:mtext><mml:mrow><mml:mn>80</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Physical Review B, 2008, 78, .	1.1	47

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55	Structural and bonding properties of bcc-based<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>B</mml:mtext><mml:mrow><mml:mn>80</mml:mn></mml:mrow></mml:m Physical Review B, 2008, 78, .	1.1	29
56	Polarizabilities of intermediate sized lithium clusters from density-functional theory. Journal of Computational Methods in Sciences and Engineering, 2008, 7, 495-505.	0.1	0
57	The static dipole polarizability of C₇₀fullerene. Journal of Physics B: Atomic, Molecular and Optical Physics, 2007, 40, 3491-3496.	0.6	18
58	Efficient quantum-chemical geometry optimization and the structure of large icosahedral fullerenes. Chemical Physics Letters, 2006, 422, 451-454.	1.2	49
59	Dipole moments from atomic-number-dependent potentials in analytic density-functional theory. Journal of Chemical Physics, 2006, 125, 214104.	1.2	3
60	The limitations of Slaterâ€™s element-dependent exchange functional from analytic density-functional theory. Journal of Chemical Physics, 2006, 124, 044107.	1.2	18
61	Momentum-space properties from coordinate-space electron density. Journal of Chemical Physics, 2005, 122, 204110.	1.2	9
62	Accurate molecular energies by extrapolation of atomic energies using an analytic quantum mechanical model. Physical Review B, 2005, 71, .	1.1	14
63	Theoretical infrared, Raman, and optical spectra of theB36N36cage. Physical Review A, 2005, 71, .	1.0	24
64	Slater's Exchange Parameters Î± for Analytic and Variational XÎ± Calculations. Journal of Chemical Theory and Computation, 2005, 1, 1193-1200.	2.3	19
65	Electronic structure of fullerenelike cages and finite nanotubes of aluminum nitride. Physical Review B, 2005, 72, .	1.1	38
66	Are hemispherical caps of boronâ€“nitride nanotubes possible?. Chemical Physics Letters, 2004, 386, 403-407.	1.2	47
67	Stability of Asn [n=4, 8, 20, 28, 32, 36, 60] cage structures. Chemical Physics Letters, 2004, 387, 476-480.	1.2	33
68	Electronic structure, vibrational stability, infra-red, and Raman spectra of B24N24 cages. Chemical Physics Letters, 2004, 393, 300-304.	1.2	50
69	On the optimal value of Î± for the Hartreeâ€“Fockâ€“Slater method. Chemical Physics Letters, 2004, 399, 417-421.	1.2	7
70	Electronic structure, vibrational stability, and predicted infrared-Raman spectra of the As[sub 20], As@Ni[sub 12], and As@Ni[sub 12]@As[sub 20] clusters. Journal of Chemical Physics, 2004, 121, 11007.	1.2	9
71	Density functional study of structural and electronic properties of NanMgâ€,(1â©½nâ©½12) clusters. Journal of Chemical Physics, 2001, 115, 2109-2116.	1.2	19
72	Momentum-space properties of atoms: Application of the generalized-gradient approximation. Physical Review A, 2000, 62, .	1.0	11

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73	Temperature Dependence of the Polarizability of Sodium Clusters. Physical Review Letters, 2000, 84, 4826-4829.	2.9	49
74	Full-potential LAPW calculation of magnetic Compton profiles of Ni. Physical Review B, 2000, 62, 16435-16441.	1.1	5
75	Full-potential LAPW calculation of electron momentum density and related properties of Li. Physical Review B, 1999, 60, 10770-10775.	1.1	16
76	Positron and positronium affinities in the work-formalism Hartree-Fock approximation. Physical Review A, 1999, 60, 218-223.	1.0	1
77	Atomic Compton profiles within different exchange-only theories. European Physical Journal D, 1999, 7, 151-155.	0.6	12
78	Total atomic energies using indirect-path methods. Physical Review A, 1996, 53, 3652-3655.	1.0	5
79	Leading corrections to the compton profiles beyond the impulse approximation: second-order correction. Chemical Physics Letters, 1995, 242, 555-559.	1.2	2
80	Positron binding: A positron-density viewpoint. Physical Review A, 1994, 50, 2191-2196.	1.0	9
81	Fully Analytic Implementation of Density Functional Theory for Efficient Calculations on Large Molecules. , 0, , 157-168.		1