Tunna Baruah

List of Publications by Year
in descending order

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61 papers	1,275 citations	304602 22 h-index	395590 33 g-index
61 all docs	61 docs citations	61 times ranked	1031 citing authors

#	Article	IF	Citations
1	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
2	DFT Calculations on Charge-Transfer States of a Carotenoid-Porphyrin-C₆₀ Molecular Triad. Journal of Chemical Theory and Computation, 2009, 5, 834-843.	2.3	62
3	Static dielectric response of icosahedral 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 an all-electron density functional theory. Physical Review B, 2008, 77, .	1.1	58
4	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
5	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
6	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
7	Stretched or noded orbital densities and self-interaction correction in density functional theory. Journal of Chemical Physics, 2019, 150, 174102.	1.2	46
8	Self-Interaction Corrections Within the Fermi-Orbital-Based Formalism. Advances in Atomic, Molecular and Optical Physics, 2015, 64, 153-180.	2.3	42
9	Density-Functional-Based Determination of Vibrational Polarizabilities in Molecules within the Double-Harmonic Approximation:â€‰ Derivation and Application. Journal of Chemical Theory and Computation, 2005, 1, 590-596.	2.3	39
10	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
11	Charge transfer excited state energies by perturbative delta self consistent field method. Journal of Chemical Physics, 2012, 137, 084316.	1.2	35
12	Self-interaction corrections applied to Mg-porphyrin, C60, and pentacene molecules. Journal of Chemical Physics, 2016, 144, 164117.	1.2	34
13	Density functional study on a light-harvesting carotenoid-porphyrin-C60 molecular triad. Journal of Chemical Physics, 2006, 125, 164706.	1.2	33
14	Fermi-LÃ¶wdin orbital self-interaction correction to magnetic exchange couplings. Journal of Chemical Physics, 2018, 149, 164101.	1.2	33
15	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
16	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
17	The effect of self-interaction error on electrostatic dipoles calculated using density functional theory. Journal of Chemical Physics, 2019, 151, 174106.	1.2	29
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	Charge transfer excitations in cofacial fullerene-porphyrin complexes. Journal of Chemical Physics, 2012, 137, 084317.	1.2	26
20	Second-order transverse magnetic anisotropy induced by disorder in the single-molecule magnetMn12. Physical Review B, 2004, 69, .	1.1	25
21	Theoretical infrared, Raman, and optical spectra of theB36N36cage. Physical Review A, 2005, 71, .	1.0	24
22	Density functional study of the conformers of Co4-based single-molecule magnet. International Journal of Quantum Chemistry, 2003, 93, 324-331.	1.0	23
23	Excited States of Light-Harvesting Systems Based on Fullerene/Graphene Oxide and Porphyrin/Smaragdyrin. Journal of Physical Chemistry C, 2017, 121, 4859-4872.	1.5	23
24	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
25	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
26	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
27	Effect of geometrical orientation on the charge-transfer energetics of supramolecular (tetraphenyl)-porphyrin/C60 dyads. Journal of Chemical Physics, 2013, 138, 074306.	1.2	20
28	The Role of Self-Interaction Corrections, Vibrations, and Spin-Orbit in Determining the Ground Spin State in a Simple Heme. Magnetochemistry, 2017, 3, 31.	1.0	18
29	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
30	Dipole polarizability of isovalent carbon and boron cages and fullerenes. Physical Review B, 2009, 80, .	1.1	16
31	Analytic atomic gradients in the fermiâ€Ã¶wdin orbital selfâ€interaction correction. Journal of Computational Chemistry, 2019, 40, 820-825.	1.5	16
32	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
33	Crystalline Alloys of Organic Donors and Acceptors Based on TIPS-Pentacene. Journal of Physical Chemistry C, 2015, 119, 20823-20832.	1.5	14
34	Local self-interaction correction method with a simple scaling factor. Physical Chemistry Chemical Physics, 2021, 23, 2406-2418.	1.3	14
35	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
36	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

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37	Geometry and electronic structure of neutral and charged B21 clusters. Chemical Physics Letters, 2013, 557, 15-18.	1.2	13
38	Static dipole polarizabilities of polyacenes using self-interaction-corrected density functional approximations. Journal of Chemical Physics, 2021, 154, 114305.	1.2	12
39	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
40	Calcium coated B80 fullerene: A study on various coating configurations of B80. Chemical Physics Letters, 2011, 514, 66-69.	1.2	11
41	Site specific atomic polarizabilities in endohedral fullerenes and carbon onions. Journal of Chemical Physics, 2015, 143, 084306.	1.2	11
42	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
43	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
44	Positron binding: A positron-density viewpoint. Physical Review A, 1994, 50, 2191-2196.	1.0	9
45	Zn(II)-Porphyrinâ€“Squaraine Dyads as Potential Components for Dye-Sensitized Solar Cells: A Quantum Chemical Study of Optical and Charge Transport Properties. Journal of Physical Chemistry C, 2020, 124, 12968-12981.	1.5	9
46	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
47	Density-related properties from self-interaction corrected density functional theory calculations. Journal of Chemical Physics, 2021, 154, 024102.	1.2	8
48	Self-interaction-corrected Kohnâ€“Sham effective potentials using the density-consistent effective potential method. Journal of Chemical Physics, 2021, 155, 064109.	1.2	8
49	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
50	Electronic and Optical Properties of VSc₂N@C₆₈ Fullerene. Journal of Physical Chemistry C, 2016, 120, 27813-27819.	1.5	7
51	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
52	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
53	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
54	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

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55	Density functional investigation of the electronic structure and charge transfer excited states of a multichromophoric antenna. Chemical Physics, 2016, 469-470, 1-8.	0.9	3
56	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
57	Excited Electronic States of Porphyrin-Based Assemblies Using Density Functional Theory. , 2016, , 233-289.		1
58	Mesomorphic Behavior in Silver(I) N-(4-Pyridyl) Benzamide with Aromatic Ï€â€“Ï€ Stacking Counterions. Materials, 2018, 11, 1666.	1.3	1
59	Density-Functional Based Investigation of Molecular Magnets. Computational Chemistry - Reviews of Current Trends, 2006, , 83-120.	0.4	1
60	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
61	Equivalence of Electron-Vibration Interaction and Charge-Induced Force Variations: A New O(1) Approach to an Old Problem. Crystals, 2012, 2, 236-247.	1.0	0