Biswajit Santra

List of Publications by Year
in descending order

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33 papers	7,086 citations	304743 22 h-index	395702 33 g-index
33 all docs	33 docs citations	33 times ranked	9269 citing authors

#	Article	IF	Citations
1	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	1.8	4,303
2	Ab initio theory and modeling of water. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 10846-10851.	7.1	340
3	The individual and collective effects of exact exchange and dispersion interactions on the ab initio structure of liquid water. Journal of Chemical Physics, 2014, 141, 084502.	3.0	276
4	Benzene adsorbed on metals: Concerted effect of covalency and van der Waals bonding. Physical Review B, 2012, 86, .	3.2	243
5	On the accuracy of density-functional theory exchange-correlation functionals for H bonds in small water clusters. II. The water hexamer and van der Waals interactions. Journal of Chemical Physics, 2008, 129, 194111.	3.0	211
6	On the accuracy of density-functional theory exchange-correlation functionals for H bonds in small water clusters: Benchmarks approaching the complete basis set limit. Journal of Chemical Physics, 2007, 127, 184104.	3.0	208
7	Hydrogen Bonds and van der Waals Forces in Ice at Ambient and High Pressures. Physical Review Letters, 2011, 107, 185701.	7.8	193
8	Hydroxide diffuses slower than hydronium in water because its solvated structure inhibits correlated proton transfer. Nature Chemistry, 2018, 10, 413-419.	13.6	175
9	To Wet or Not to Wet? Dispersion Forces Tip the Balance for Water Ice on Metals. Physical Review Letters, 2011, 106, 026101.	7.8	159
10	Structure and energetics of benzene adsorbed on transition-metal surfaces: density-functional theory with van der Waals interactions including collective substrate response. New Journal of Physics, 2013, 15, 053046.	2.9	143
11	On the accuracy of van der Waals inclusive density-functional theory exchange-correlation functionals for ice at ambient and high pressures. Journal of Chemical Physics, 2013, 139, 154702.	3.0	119
12	Local structure analysis in ab initio liquid water. Molecular Physics, 2015, 113, 2829-2841.	1.7	96
13	Coupled cluster benchmarks of water monomers and dimers extracted from density-functional theory liquid water: The importance of monomer deformations. Journal of Chemical Physics, 2009, 131, 124509.	3.0	62
14	Structural, electronic, and dynamical properties of liquid water by ab initio molecular dynamics based on SCAN functional within the canonical ensemble. Journal of Chemical Physics, 2018, 148, 164505.	3.0	58
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.	7.1	57
16	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. Journal of Chemical Physics, 2019, 151, 214108.	3.0	56
17	Isotope effects in liquid water via deep potential molecular dynamics. Molecular Physics, 2019, 117, 3269-3281.	1.7	52
18	A systematic study of chloride ion solvation in water using van der Waals inclusive hybrid density functional theory. Molecular Physics, 2015, 113, 2842-2854.	1.7	47

#	Article	IF	Citations
19	Stretched or noded orbital densities and self-interaction correction in density functional theory. Journal of Chemical Physics, 2019, 150, 174102.	3.0	46
20	Perdew-Zunger self-interaction correction: How wrong for uniform densities and large-Z atoms?. Journal of Chemical Physics, 2019, 150, 174106.	3.0	35
21	Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory Based Ab Initio Molecular Dynamics. 1. Theory, Algorithm, and Performance. Journal of Chemical Theory and Computation, 2020, 16, 3757-3785.	5.3	29
22	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.	3.0	23
23	In situ Characterization of Nanoparticles Using Rayleigh Scattering. Scientific Reports, 2017, 7, 40230.	3.3	22
24	Isotope effects in molecular structures and electronic properties of liquid water via deep potential molecular dynamics based on the SCAN functional. Physical Review B, 2020, 102, .	3.2	22
25	Root-growth of boron nitride nanotubes: experiments and ab initio simulations. Nanoscale, 2018, 10, 22223-22230.	5.6	19
26	Thermal expansion in dispersion-bound molecular crystals. Physical Review Materials, 2018, 2, .	2.4	18
27	Self-interaction correction in waterâ€“ion clusters. Journal of Chemical Physics, 2021, 154, 094302.	3.0	16
28	The Fermiâ€“LÃ¶wdin self-interaction correction for ionization energies of organic molecules. Journal of Chemical Physics, 2020, 153, 184303.	3.0	12
29	Exploring and enhancing the accuracy of interior-scaled Perdewâ€“Zunger self-interaction correction. Journal of Chemical Physics, 2021, 154, 094105.	3.0	12
30	X-ray absorption of liquid water by advanced ab initio methods. Physical Review B, 2017, 96, .	3.2	11
31	Simple hydrogenic estimates for the exchange and correlation energies of atoms and atomic ions, with implications for density functional theory. Journal of Chemical Physics, 2020, 153, 074114.	3.0	10
32	Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory-Based Ab Initio Molecular Dynamics II: Extensions to the Isobaricâ€“Isoenthalpic and Isobaricâ€“Isothermal Ensembles. Journal of Chemical Theory and Computation, 2021, 17, 7789-7813.	5.3	7
33	Isotope effects in x-ray absorption spectra of liquid water. Physical Review B, 2020, 102, .	3.2	6