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Exchange-correlation hole of a generalized gradient approximation for solids and surfaces

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#	Paper	IF	Citations
45	Exchange-correlation energy functional based on the Airy-gas reference system. <i>Physical Review B</i> , 2009 , 80,	3.3	15
44	Gradient-dependent density functionals of the Perdew-Burke-Ernzerhof type for atoms, molecules, and solids. <i>Physical Review B</i> , 2009 , 79,	3.3	31
43	Generalized gradient approximation bridging the rapidly and slowly varying density regimes: A PBE-like functional for hybrid interfaces. <i>Physical Review B</i> , 2010 , 82,	3.3	46
42	Global Hybrid Functionals: A Look at the Engine under the Hood. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 3688-3703	6.4	77
41	Relativity and the lead-acid battery. <i>Physical Review Letters</i> , 2011 , 106, 018301	7.4	80
40	Relativity and the mercury battery. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 16510-2	3.6	13
39	Improving atomization energies of molecules and solids with a spin-dependent gradient correction from one-electron density analysis. <i>Physical Review B</i> , 2011 , 84,	3.3	23
38	Correlation energy functional from jellium surface analysis. <i>Physical Review B</i> , 2011 , 84,	3.3	36
37	Review on the Properties of Nano-/Microstructures in the Catalyst Layer of PEMFC. <i>Journal of Fuel Cell Science and Technology</i> , 2011 , 8,		16
36	Improved hybrid functional for solids: the HSEsol functional. <i>Journal of Chemical Physics</i> , 2011 , 134, 024116	3.6	240
35	Spin-dependent gradient correction for more accurate atomization energies of molecules. <i>Journal of Chemical Physics</i> , 2012 , 137, 194105	3.9	21
34	Semilocal dynamical correlation with increased localization. <i>Physical Review B</i> , 2012 , 86,	3.3	39
33	Interlayer potentials for fcc (1 1 1) planes of PdAg random alloys. <i>Computational Materials Science</i> , 2012 , 63, 20-27	3.2	11
32	Testing the broad applicability of the PBEint GGA functional and its one-parameter hybrid form. <i>International Journal of Quantum Chemistry</i> , 2013 , 113, 673-682	2.1	29
31	Modeling development on the meso-scale reacting transport phenomena in proton exchange membrane fuel cells. <i>Acta Mechanica Sinica/Lixue Xuebao</i> , 2013 , 29, 370-378	2	1
30	Relevance of coordinate and particle-number scaling in density-functional theory. <i>Physical Review A</i> , 2013 , 87,	2.6	34
29	Construction of a general semilocal exchange-correlation hole model: Application to nonempirical meta-GGA functionals. <i>Physical Review B</i> , 2013 , 88,	3.3	37

28	Interpretation of van der Waals density functionals. <i>Physical Review B</i> , 2014 , 90,	3.3	57
27	Paradox of Self-Interaction Correction. <i>Advances in Atomic, Molecular and Optical Physics</i> , 2015 , 1-14	1.7	21
26	Electronic Structure and Transport Properties of Doped Lead Chalcogenides from First Principles. <i>MRS Advances</i> , 2016 , 1, 4003-4010	0.7	1
25	Kinetic-energy-density dependent semilocal exchange-correlation functionals. <i>International Journal of Quantum Chemistry</i> , 2016 , 116, 1641-1694	2.1	62
24	Predicting single phase CrMoWX high entropy alloys from empirical relations in combination with first-principles calculations. <i>Intermetallics</i> , 2017 , 83, 9-16	3.5	15
23	Properties of real metallic surfaces: Effects of density functional semilocality and van der Waals nonlocality. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, E9188-E9196	11.5	105
22	A meta-GGA level screened range-separated hybrid functional by employing short range Hartree-Fock with a long range semilocal functional. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 8999-9005	3.6	17
21	Assessing the performance of the recent meta-GGA density functionals for describing the lattice constants, bulk moduli, and cohesive energies of alkali, alkaline-earth, and transition metals. <i>Journal of Chemical Physics</i> , 2018 , 149, 164703	3.9	19
20	Dispersion-corrected PBEsol exchange-correlation functional. <i>Physical Review B</i> , 2018 , 98,	3.3	26
19	Efficient lattice constants and energy bandgaps for condensed systems from a meta-GGA level screened range-separated hybrid functional. <i>Journal of Chemical Physics</i> , 2018 , 149, 094105	3.9	10
18	Assessing the performance of the Tao-Mo semilocal density functional in the projector-augmented-wave method. <i>Journal of Chemical Physics</i> , 2018 , 149, 044120	3.9	32
17	Solid-State Testing of a Van-Der-Waals-Corrected Exchange-Correlation Functional Based on the Semiclassical Atom Theory. <i>Computation</i> , 2018 , 6, 7	2.2	14
16	Efficient band gap prediction of semiconductors and insulators from a semilocal exchange-correlation functional. <i>Physical Review B</i> , 2019 , 100,	3.3	24
15	Screened hybrid meta-GGA exchange-correlation functionals for extended systems. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 3002-3015	3.6	9
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13	Improved transition metal surface energies from a generalized gradient approximation developed for quasi two-dimensional systems. <i>Journal of Chemical Physics</i> , 2020 , 152, 151101	3.9	5
12	Computational determination of coordination structure impact on adsorption and acidity of pristine and sulfated MOF-808. <i>Materials Advances</i> , 2021 , 2, 4246-4254	3.3	4
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9	GPU_PBTE: an efficient solver for three and four phonon scattering rates on graphics processing units. <i>Journal of Physics Condensed Matter</i> , 2021 , 33,	1.8	3
8	vdW-DF-ahcx: a range-separated van der Waals density functional hybrid. <i>Journal of Physics Condensed Matter</i> , 2021 , 34,	1.8	2
7	A way of resolving the order-of-limit problem of Tao-Mo semilocal functional. <i>Journal of Chemical Physics</i> , 2020 , 153, 184112	3.9	6
6	Engineering Periodic Dinuclear Lanthanide-Directed Networks Featuring Tunable Energy Level Alignment and Magnetic Anisotropy by Metal Exchange.. <i>Small</i> , 2022 , e2107073	11	1
5	First-principles study of the electrical resistivity in zirconium dichalcogenides with multivalley bands: Mode-resolved analysis of electron-phonon scattering. <i>Physical Review B</i> , 2021 , 104,	3.3	1
4	Theoretical insights on structural, mechanical and thermodynamic properties of MCoB (M=Nb, Mo, and W) ternary borides under high pressure. <i>Solid State Sciences</i> , 2022 , 106931	3.4	0
3	Prediction of the pressure-induced phase transition, mechanical properties, and electronic structures for ScB4 via first principle calculations. <i>Applied Physics A: Materials Science and Processing</i> , 2022 , 128,	2.6	
2	Solvent extraction of vanadium with D2EHPA from aqueous leachate of stone coal after low temperature sulfation roasting. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022 , 650, 129584	5.1	2
1	First-principles calculations to investigate strain effects on structural, electronic, elastic and transport properties of Cs2PdBr6. 2022 , 1215, 113833		0