Regularized Gradient Expansion for Atoms, Molecules, and Solids

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#	Paper	IF	Citations
35	Insight into the performance of GGA functionals for solid-state calculations. *Physical Review B*, **2009**, 80,	3.3	59
34	Unified Inter- and Intramolecular Dispersion Correction Formula for Generalized Gradient Approximation Density Functional Theory. *Journal of Chemical Theory and Computation*, **2009**, 5, 2950-8	6.4	70
33	Generalized gradient approximation bridging the rapidly and slowly varying density regimes: A PBE-like functional for hybrid interfaces. *Physical Review B*, **2010**, 82,	3.3	46
32	Stability of Hydrocarbons of the Polyhedrane Family Containing Bridged CH Groups: A Case of Failure of the Colle-Salvetti Correlation Density Functionals. *Journal of Chemical Theory and Computation*, **2010**, 6, 3442-55	6.4	16
31	Global Hybrid Functionals: A Look at the Engine under the Hood. *Journal of Chemical Theory and Computation*, **2010**, 6, 3688-3703	6.4	77
30	Iron porphyrins with different imidazole ligands. A theoretical comparative study. *Journal of Physical Chemistry A*, **2010**, 114, 9554-69	2.8	45
29	Construction of an optimal GGA functional for molecules and solids. *Physical Review B*, **2011**, 83,	3.3	71
28	Two-Dimensional Scan of the Performance of Generalized Gradient Approximations with Perdew-Burke-Ernzerhof-Like Enhancement Factor. *Journal of Chemical Theory and Computation*, **2011**, 7, 3548-59	6.4	46
27	Improving atomization energies of molecules and solids with a spin-dependent gradient correction from one-electron density analysis. *Physical Review B*, **2011**, 84,	3.3	23
26	Correlation energy functional from jellium surface analysis. *Physical Review B*, **2011**, 84,	3.3	36
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16	Optimized Exchange and Correlation Semilocal Functional for the Calculation of Energies of Formation. *Journal of Chemical Theory and Computation*, **2015**, 11, 3844-50	6.4	18
15	Accurate Diels-Alder reaction energies from efficient density functional calculations. *Journal of Chemical Theory and Computation*, **2015**, 11, 2879-88	6.4	17
14	Rungs 1 to 4 of DFT Jacobs ladder: Extensive test on the lattice constant, bulk modulus, and cohesive energy of solids. *Journal of Chemical Physics*, **2016**, 144, 204120	3.9	142
13	Visualization and analysis of the Kohn-Sham kinetic energy density and its orbital-free description in molecules. *Journal of Chemical Physics*, **2016**, 144, 084107	3.9	22
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7	Seeking an accurate generalized-gradient approximation functional for high pressure molecular fluids. *Journal of Applied Physics*, **2017**, 122, 185902	2.5	6
6	Simple Modifications of the SCAN Meta-Generalized Gradient Approximation Functional. *Journal of Chemical Theory and Computation*, **2018**, 14, 2469-2479	6.4	23
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4	Control of surface reactivity towards unsaturated C C bonds and H over Ni-based intermetallic compounds in semi-hydrogenation of acetylene. *Journal of Catalysis*, **2019**, 372, 151-162	7.3	9
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