SCAN+*r*VV10: A van der Waals density functional for layered materials and more

Mean Absolute Relative Errors (%)			
Methods	E_b	c	a
vdW-DF1	20	7.7	2.5
optPBE-DF1	12	1.4	4.4
optB88-DF1	23	1.0	1.9
optB86b-DF1	27	0.6	1.0
cx-DF1	22	0.9	0.9
vdW-DF2	15	5.8	4.2
revB86b-DF2	16 (26)	0.6	0.9
VV10	53	1.8	1.8
SCAN	61	4.4	0.6
SCAN+*r*VV10	8	1.4	0.6

Mean absolute relative errors in percentage for interlayer binding energy, inter- and intra-layer lattice constants for 28 layered materials of SCAN+*r*VV10, compared with various van der Waals density functionals.

H. Peng, Z.-H. Yang, J. P. Perdew, and J. Sun, *Phys. Rev. X 6, 041005.* DOI: 10.1103/PhysRevX.6.041005.

Work performed at Temple University

Scientific Achievement

With SCAN+*r*VV10, we further expand the capability of the recent developed strongly constrained appropriately normed (SCAN) meta-generalized gradient approximation to the van der Waals region, by seamlessly supplying the non-local correlation functional from *r*VV10.

Significance and Impact

SCAN+*r*VV10 provides an accurate and efficient description for covalent, ionic, metallic, and van der Waals bonding on the same footing. For layered materials, which are the main subject of our center, SCAN+*r*VV10 is the first functional with the mean absolute relative errors <10%, < 2%, <1% for the interlayer binding, spacing, and the intralayer lattice constants. SCAN+*r*VV10 also inherits the excellent performance of SCAN for solids, etc.

Research Details

We implemented the *r*VV10 method within VASP, determined the parameter which joins SCAN and *r*VV10, and demonstrated the versatility of the resultant SCAN+*r*VV10 functional with 22 molecular dimers, 50 solids, benzene and graphene adsorption on metal surfaces, rare gas solids, and 28 layered materials.

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