Max-Planck-Institut für Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter

Thursday, April 12th, 2018 – 14:00 a.m.
CFEL Seminar room III (Bldg. 99)

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Orbital-dependent improvements to density-functional approximations: Application of the FLO-SIC method

The accuracy of density functional theory (DFT) calculations is limited by the so called self-interaction error [1]. The recently proposed Fermi-Löwdin orbital based method [2,3,4] for self-interaction correction (FLO-SIC) is a unitary invariant and size extensive approach to overcome this error. The current state of the method as implemented in the NRLMOL program package is presented and the performance of FLO-SIC DFT applied to atoms and molecules is discussed. The FLO-SIC method restores the correct -1/r behaviour together with the atomic infinity limit
for bond dissociation and exhibits the energy derivative discontinuity.
In addition this method delivers a description of the chemical bonding as intuitive as Lewis theory that may bridge the gap between DFT and chemical intuition.

[1] J. P. Perdew, A. Zunger, Phys. Rev. B 23, 5048 (1981)
[2] M. R. Pederson et al., J. Chem. Phys., vol. 140, 121103 (2014)
[3] M. R. Pederson, J. Chem. Phys., vol. 142, 064112 (2015)
[4] T. Hahn et. al., J. Chem. Phys., vol- 143, 224104 (2015)

Host: Angel Rubio

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