NRLMOL Tutorials and Documentation Documentation

Release 0

NRLMOL users

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CHAPTER

ONE

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1.1 Introduction and Overview

The FLOSIC code is based on the UTEP version of the NRLMOL code, the Naval Research Laboratory Molecular Orbital Library.[1]_[2][3][4] It contains an implementation of the Fermi-Löwdin orbital self-interaction correction (FLO-SIC) method[5][6][7][8] , a method to correct the self-interaction error of common exchange-correlation functionals. The underlying NRLMOL code is a massively parallel code for electronic structure calculations on molecules and clusters. It is based on the Kohn-Sham (KS) formulation of density functional theory (DFT) and solves KS equations by expressing the KS orbitals as a linear combination of Gaussian orbitals. NRLMOL is principally developed by Mark Pederson and collaborators.

In FLO-SIC, the Kohn-Sham orbitals are transformed into Fermi orbitals, which are orthogonalized to become Fermi-Löwdin orbitals (FLOs). These FLOs are used to evaluate the orbital-dependent self-interaction correction. The transformation uses points in space, the so-called Fermi-orbital descriptors (FODs). These FODs form the electronic geometry, which needs to be optimized to obtain the right FLOs and with that the correct SIC. Thus, there are two geometries to consider: The molecular geometry (given by the atoms) and the electronic geometry (given by the FODs). The optimization of the FODs is a crucial part of any FLO-SIC calculation and needs to be done carefully to get reasonable answers. For any FLO-SIC calculation, an initial set of FODs is optimized until the total energy and the FOD forces are converged. Further details about FODs are discussed in section 1.7 of this manual.

Here is a list of some SIC related properties that are calculated using the FLOSIC code:

- Total energy
- SIC energy
- Orbital energies
- Contributions to the orbital energies
- Atomic forces with SIC Pulay forces
- Analytical FOD forces for FOD optimization
- Available optimizers: conjugate gradient, LBFGS

[2] K.A. Jackson and M.R. Pederson, *Phys. Rev. B*, **42**, 3276, 1990.

[3] D. Porezag and M.R. Pederson, *Phys. Rev. A*, **60**, 2840, 1999.

[4] M. R. Pederson et al., *Phys. Stat. Sol. b*, **217**, 197, 2000.

[5] M.R. Pederson, A. Ruzsinszky, J.P. Perdew., *J. Chem. Phys.*