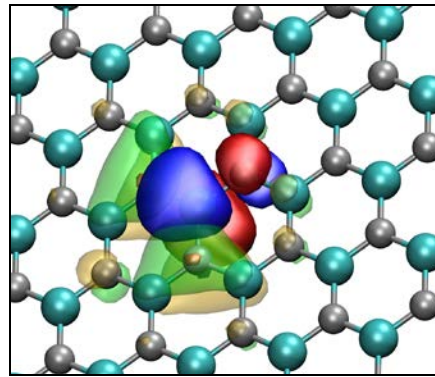


Quantum Embedding



Gustavo E. Scuseria



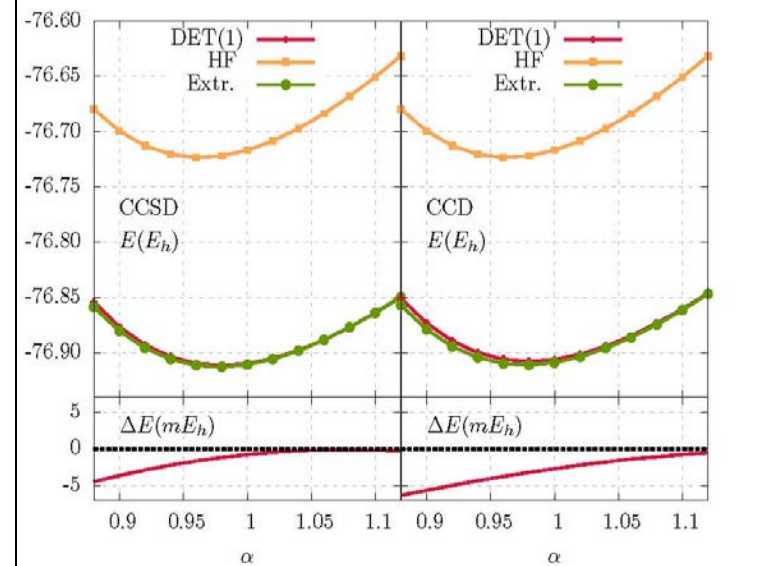
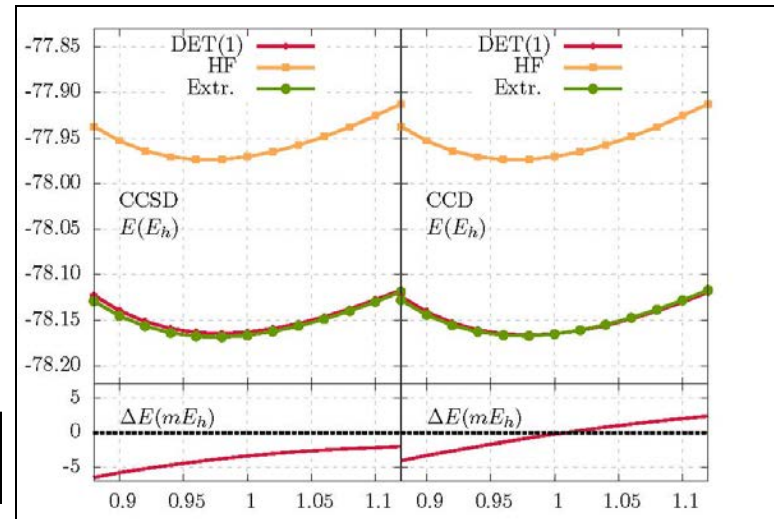
Example of fragment (red & blue) and bath (green & yellow) orbitals in BN 2D lattice

Key features

- Truncation of electronic degrees of freedom to locally important active space
- Formation of impurity Hamiltonian with small number of single particle states
- Introduction of bath states emulating the environment of the fragment

Challenges to address

- Broad benchmark of quantum chemical tools applicable as impurity solvers
- Benchmark of the method for large set of periodic systems
- Efficient implementation of impurity Hamiltonian by employing symmetry
- Developing methodology for accessing properties beyond energy and energy derivatives



Energy as a function of uniform stretching parameter α for $-(\text{CH}_2\text{-CH}_2)-$ (top) and $-(\text{CH}=\text{CH})-$ (bottom). Single cell DET compares favorably with extrapolated data for CCD and CCSD impurity solver.