Order-N quantum chemistry Package for large scale *ab initio* Simulation

HONPAS

Version 1

November, 2013

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Contents

1 INTRODUCTION

HONPAS is based on SIESTA, but adding:

- Density matrix purification methods to make construction of the density matrix in $O(N)$ operations
- Maximally localized Wannier functions
- Density-matrix perturbation theory
- Hartree-Fock method for molecule or solid
- Hybrid functionals: B3LYP, PBE0, HSE06 for molecule or solid
- MP2 method for molecule or solid
- All the new feathers are compiled for serial or parallel execution (under MPI).

References:

- "Spin-unrestricted linear-scaling electronic structure theory and its application to magnetic carbon-doped boron nitride nanotubes"

  Xiang, HJ, Liang, WZ, Yang, JL, Hou, JG and Zhu, QS. J. Chem. Phys., **123**, 124105 (2005)

  Density matrix purification methods implemented in HONPAS

- "Linear scaling calculation of maximally localized Wannier functions with atomic basis set"

  Xiang, HJ, Yang, JL, Hou, JG and Zhu, QS. J. Chem. Phys., **126**, 244707 (2007)

  Calculation of maximally localized Wannier functions in HONPAS

- "Linear-scaling density matrix perturbation treatment of electric fields in solids"

  Xiang, HJ, Yang, JL, Hou, JG and Zhu, QS. Phys. Rev. Lett., **97**, 266402 (2006)

  Density matrix perturbation theory implemented in HONPAS

- "Implementation of Exact Exchange with Numerical Atomic Orbitals" H. H. Shang, Z. Y. Li, and J. L. Yang, J. Phys. Chem. A 114, 1039 (2010)

  HF and B3LYP in HONPAS

- "Implementation of screened hybrid density functional for periodic systems with numerical atomic orbitals: Basis function fitting and integral screening" H. H. Shang, Z. Y. Li, and J. L. Yang, J. Chem. Phys. **135**, 034110 (2011)

  HSE06 in HONPAS

- "Linear scaling electronic structure calculations with numerical atomic basis set"

  H. H. Shang, Z. Y. Li, and J. L. Yang, Int. Rev. Phys. Chem. **29**, 665 (2010).

  Review for O(N) method with numerical atomic basis set

2 COMPILATION

If you just want to compile the program, go to `Obj` and issue the command:

```
sh ../Src/obj_setup.sh
```

Then use:

```
make HONPAS
```

The executable should work for any job.

3 DETAILED DESCRIPTION OF PROGRAM OPTIONS

As we based on SIESTA, the input files are the same except the following:

3.1 Order(N) calculations

ON purification Choice of purification method

- `TC2`

3.2 Maximally localized Wannier functions

MLWF Generate maximally localized Wannier functions for molecules.

3.3 Hartree-Fock for exact exchange energy

HF (*string*): Make a Hartree-Fock calculation for molecule or solid

- `numeric` Using isf-poisson solver to calculate ERI numerically.
- `NAO2GTO` Using more efficient NAO2GTO scheme to calculate ERI.

Default value: `NAO2GTO`

3.4 Hybrid Exchange-correlation functionals

XC.functional (*string*): Exchange-correlation functional type. As we add hybrid functionals, so the default is `GGA` (Generalized Gradient Approximation).

Default value: `GGA`

XC.authors (*string*): Particular parametrization of the exchange-correlation functional. Options are:

- `B3LYP`
  Ref: Becke, A. D. J. Chem. Phys. **98**, 5648 (1993)
- `HSE06`
  Ref: A. V. Krukau, O. A. Vydrov, A. F. Izmaylov and G. E. Scuseria, J. Chem. Phys. **125**, 224106 (2006).

Default value: `HSE06`

3.5 Second-order MøllerPlesset perturbation for correlation energy

MP2 Make a Hartree-Fock calculation for molecule or solid.

Default value: `MP2`