

Hybrids in ABINIT

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The status of the implementation of hybrids in ABINIT will be reviewed. The Fock exchange term, the PBE0, B3LYP and HSE functionals, are implemented both in the norm-conserving pseudopotential framework and in the PAW one, in the non-spin-polarized and spin-polarized cases. In all these cases, forces and stresses are computed. Also, the wavefunctions that are obtained in the norm-conserving case can be used as a starting point to perform GW calculations. The implementation for spinor wavefunctions is not yet available.

Work is still in progress concerning the efficiency of the calculation. The adaptively compressed exchange operator [1] is implemented, giving typically a 3-4 speedup. Fock operator k-point downsampling [2] and parallelism is available. A double-loop algorithm, including wavefunction mixing through biorthogonalization, is under development.

References

- [1] Lin Lin, J. Chem. Theory Comput. **12**, 2242 (2016).
- [2] J. Paier et al, J. Chem. Phys. **124**, 154709 (2006).