Periodic MRChem

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MRChem is a numerical real-space code for molecular electronic structure calculations within the self-consistent field (SCF) approximation of quantum chemistry, Hartree–Fock and Density Functional Theory. MRChem uses a multiwavelet (MW) basis, and are used in quantum chemical calculations due to their mathematical properties, such as, error control and low scaling. The code has recently been applied to two large and precise benchmark studies on electronic energies[1] and magnetizabilities and shielding constants[2].

We are currently expanding the code to solve the Kohn–Sham equations for crystalline systems. We give an overview of this work including examples of total energies compared with other solid state codes, and how MWs can be used to systematically increase the accuracy of the result with respect to the basis set.

References

1. S. R. Jensen, S. Saha, J. A. Flores-Livas, W. Huhn, V. Blum, S. Goedecer, and L. Frediani, J *Phys. Chem. Lett. 8*, **1449–1457** (2017). 2. S. R. Jensen, T. Fla, D. Jonsson, R. S. Monstad, K. Ruud, and L. Frediani, *Phys. Chem. Chem. Phys. 18*, **21145–21161** (2016).