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Productive Large Scale QM Calculations

Wednesday 22 March 2023 11:10 (10 minutes)

Density Functional Theory (DFT) is a popular Quantum Mechanical framework for computing the properties of molecules and materials. Recent advances in linear-scaling algorithms and computing power have made it possible to apply DFT to systems of an unprecedented size. This has significant consequences for the research paradigms employed by DFT users. In this talk, we will precent our research on practical calculations of large systems. In particular, we will give an overview of our high-level Python interface that is able to construct complex systems, launch calculations on remote supercomputers, and decompose complex systems into core building blocks. We hope that this work may stimulate some discussion about applications of large-scale QM modelling as well as general calculation frameworks for managing calculations across multiple computing resources.

Ratcliff, Laura E., William Dawson, Giuseppe Fisicaro, Damien Caliste, Stephan Mohr, Augustin Degomme, Brice Videau et al. “Flexibilities of wavelets as a computational basis set for large-scale electronic structure calculations.” The Journal of chemical physics 152, no. 19 (2020): 194110.

JLESC topic

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