Solving strongly correlated electrons of real systems with quantum computing: application to oxydes

Context Atomic scale simulations play a central role to understand and anticipate the ageing of materials for low-carbon energy such as batteries or steels inside nuclear reactors. The successful Density Functional Theory is the state-of-the-art method to tackle these bulk materials but still fails to reach physically interesting phenomena such as paramagnetism in austenitic steels or strongly correlated electrons in oxydes. Meanwhile, quantum computing is foreseen to solve industrial materials problems but algorithms developed today in the Noisy Intermediate Scale Quantum (NISQ) era have only been tested on small or toy models. In addition, the ultimate goal of outperforming classical algorithms benefiting from dozen of years of optimisation is still out of reach.

Description of the internship In this internship, we will combine advanced quantum chemistry methods (embedding methods such as Density Matrix Embedding Theory-DMET) and quantum computing where the solving part will be a quantum algorithm that can be run on a quantum computer. Your work will be to design an innovative approach namely the quantum embedding method to solve NiO oxyde such as in (Cao et al., 2023) and to compare numerical results of this algorithm with best classical methods. The effect of noise might be explored. This internship is planned to be pursued in a PhD CIFRE.

Requirements

- Appealing for multi-disciplinary projects.
- Strong taste for Numerical work (Python, Quantum packages).
- Strong background in Quantum Mechanics, Statistical Physics, Condensed Matter Physics/Quantum Chemistry.

Logistic

- The internship will take place at EDF R&D at Moret sur Loing, near Fontainebleau (line R from Paris Gare de lyon).
- Duration is expected to be 5 to 6 months, a compensation is planned.
- Collaboration between EDF (Antoine Michel and Christophe Domain), the Montpellier University (Bruno Senjean) and Bordeaux University (Matthieu Saubanère).

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References

Cao, C., Sun, J., Yuan, X., Hu, H.-S., Pham, H. Q., & Lv, D. (2023). Ab initio quantum simulation of strongly correlated materials with quantum embedding. *npj Computational Materials*, *9*. https://doi.org/10.1038/s41524-023-01045-0

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