

What can quantum computers do for materials science?

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Quantum computers have been heralded as promising computing architectures for advancing the field of materials science.

In this talk, I will give an overview of what quantum computing can (and cannot) do for materials science, with a focus on Noisy, Intermediate Scale Quantum (NISQ) computers. In particular, I will describe the hybrid quantum classical approaches that are taken to leverage these processors despite their defects. This will range from techniques to choose an optimal basis to perform the quantum computation [1], to adaptive methods to construct quantum variational states [2]. I will also give a many-body perspective on the recent claims of quantum supremacy using the density matrix renormalization algorithm, an algorithm that is widely used to study strongly-correlated materials [3].

[1] P. Besserve, TA, Phys Rev B 22, 105, 115108

[2] M. Haidar, M. Rancic, TA, Y. Maday, J.P. Piquemal, arXiv :2206.08798

[3] TA, T. Louvet, Y. Zhou, C. Lambert, E.M. Stoudenmire, X. Waintal, arXiv :2207.05612