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Scalable machine learning for predicting the electronic structure in many-particle systems

In this presentation, I will present our recent progress in integrating machine learning to significantly boost the computational efficiency of electronic structure calculations [1]. I will specifically address our efforts to speed up density functional theory calculations, for which we have developed the Materials Learning Algorithms framework [2]. Our findings illustrate significant improvements in calculation speed for metals at their melting point. Additionally, our use of automated machine learning has yielded significant reductions in computational resources required to identify optimal neural network architectures, laying the groundwork for extensive investigations [3]. Furthermore, I will show the transferability of our ML model across temperatures [4]. Most importantly, I will present our latest breakthrough, which enables fast neural-network driven electronic structure calculations for systems unattainable by conventional density functional theory calculations [5].

References

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