Contribution ID: **39** Type: **not specified**

Accelerating Kohn-Sham Density Functional Theory with Neural Networks

Thursday 15 September 2022 11:30 (45 minutes)

Artificial intelligence (AI) has great potential for accelerating electronic structure calculations to hitherto unattainable scales [1]. I will present our recent efforts on accomplishing speeding up Kohn-Sham density functional theory calculations at finite temperatures with deep neural networks in terms of our Materials Learning Algorithms framework [2,3] by illustrating results for metals across their melting point. Furthermore, our results towards automated machine learning save orders of magnitude in computational efforts for finding suitable neural networks and set the stage for large-scale AI-driven investigations [4]. Finally, I will conclude with a preview of our most recent result that enables neural-network-driven electronic structure calculations for systems containing more than 100,000 atoms.

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Session Classification: Morning Session (Thursday)