Contribution ID: **36** Type: **not specified**

Physics-Informed Neural Networks for Quantum Dynamics of Electrons

Thursday 15 September 2022 11:00 (30 minutes)

Time-dependent density functional theory (TDDFT) is an important method for simulating dynamical processes in quantum many-body systems. We explore the feasibility of physics-informed neural networks as a surrogate for TDDFT. We examine the computational efficiency and convergence behaviour of these solvers to state-of-the-art numerical techniques on models and small molecular systems. The method developed here has the potential to accelerate the TDDFT workflow, enabling the simulation of large-scale calculations of electron dynamics in matter exposed to strong electromagnetic fields, high temperatures, and pressures.

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Session Classification: Morning Session (Thursday)