Neural quantum states for many-body electronic structure and dynamics

Giuseppe Carleo,
EPFL (Switzerland)

Abstract: This talk presents recent advances in using neural-network parameterizations of many-body wave functions for ab initio electronic structure calculations. We introduce a message-passing neural network ansatz for simulating strongly interacting electrons in continuous space, demonstrating its high accuracy for the homogeneous electron gas problem and for the unitary Fermi gas. The approach's potential for other periodic systems and materials will be discussed. Additionally, we explore the application of neural wave functions to the challenging case of many-body electronic quantum dynamics, showcasing results for quantum dots and molecules in strong laser fields.