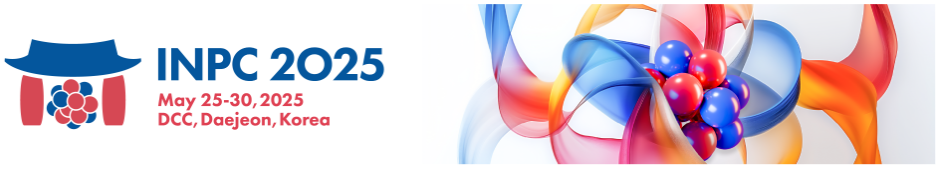


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# Nuclear orbital-free energy density functionals from machine learning

Research on quantum many-body problems is essential in a wide variety of scientific fields. By reducing the many-body problem formulated in terms of N-body wave functions to the one-body level with the density distributions, the density functional theory (DFT) has been enormously popular. However, the quality of the DFT results crucially depends on the accuracy of the energy density functional, whose existence was proved by the Hohenberg-Kohn theorem, but the actual form is unknown and has to be determined with approximations. Therefore, the present applications of DFT in nuclear physics are mainly based on orbital-based method, e.g., Kohn-Sham scheme. Practical orbital-free DFT in nuclear physics has become a big dream and challenge.

Machine learning is a powerful tool for finding existing and complicated patterns in high-dimensional data, which is very suitable for constructing the energy density functional, i.e., a functional that is proven to exist but of unknown form. In this work, machine learning is employed to build an orbital-free energy density functional for self-bound nuclear systems for the first time. By learning the kinetic energy as a functional of the nucleon density alone, a robust and accurate orbital-free density functional for nuclei is established. Self-consistent calculations that bypass the Kohn-Sham equations provide the ground-state densities, total energies, and root-mean-square radii with a high accuracy in comparison with the Kohn-Sham solutions. No existing orbital-free density functional theory comes close to this performance for nuclei. Therefore, it provides a new promising way for future developments of nuclear energy density functionals for the whole nuclear chart.

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