Artificial neural networks for the kinetic energy functional of non-interacting fermions

Thomas D. Kühne[1,2]

[1]*Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf, 02826 Görlitz, Germany*
[2]*Institute of Artificial Intelligence, Chair of Computational System Sciences, Technische Universität Dresden, 01187 Dresden, Germany*

A novel approach to find the fermionic non-interacting kinetic energy functional with chemical accuracy using machine learning techniques is presented [1]. To that extent, we apply machine learning to an intermediate quantity rather than targeting the kinetic energy directly. We demonstrate the performance of the method for three model systems containing three and four electrons. The resulting kinetic energy functional remarkably accurately reproduces self-consistently the ground state electron density and total energy of reference Kohn-Sham calculations with an error of less than 5 mHa. This development opens a new avenue to advance orbital-free density functional theory by means of machine learning.

[1] S. A. Ghasemi and T. D. Kühne, J. Chem. Phys. **154**, 074107 (2021).