

# Semi-local deep-learning kinetic energy density functional based on fourth order gradient expansion

Luis Rincón

*Universidad San Francisco de Quito, Grupo de Química Computacional y Teórica, Colegio Politécnico de Ciencias e Ingeniería, Diego de Robles y Vía Interoceánica, Quito 17-1200-841, Ecuador*

A semi-local kinetic energy density functional was constructed using a deep learning network (DLN). The present scheme employ normalized functions calculated from the fourth-order gradient expansion of the kinetic energy functionals as the explanatory variables in a DLN and the enhancement factor calculated from the Kohn-Sham kinetic energy as the response variable. DLN is able to generate an implicit kinetic energy density functional using an enormous number of data points. Numerical tests were performed in two datasets. The first dataset contains 54 atomic systems from H to Xe. A total data points of 1799890 were divided into 20% for training, 20% for validation and 60% for testing. After training, the mean absolute percentage error for the kinetic energy density is 0.042%, and the average total kinetic energy error is 7.9 mHar. The second dataset involve 200 molecules from the GDB-9 dataset. The total number of data points was 4700380 (10% for training, 10% for validation and 80% for testing). The average kinetic energy error was 15.22 mHar in the molecular dataset. The descriptors and kinetic energy density were calculated at the M06XD/6-31G\* level. The result show that the combination of Adam and AdaGrad algorithms is essential in order to obtain chemical accuracy in the total kinetic energy. The present approach reproduced the KS kinetic energy with several types of chemical bonds.