Title: Pathways to Obtain Ground State Electron Densities and Total Energies of Atomistic Systems by Means of Machine Learning Techniques

Abstract: The realm of ab initio methods to calculate total energies and other ground-state properties of atomistic systems are in practice limited to small systems due to their scaling complexities. Density functional theory (DFT) is an approximate method but the best trade-off between computational cost and accuracy. Nevertheless, DFT computation time grows cubically with system size, thereby physically relevant time and length scales are computationally too demanding. In recent years, there has been a surge in utilizing machine learning techniques to obtain an accurate treatment of interactions in many-body systems at the cost of ab initio methods. These methods can be classified into two categories, (i) algorithms that are solely based on mathematical models by neglecting the underlying physical interactions, (ii) techniques that apply machine learning algorithms to predict intermediate physical quantities or parameters in a physically relevant model Hamiltonian. We briefly review the first class and present two pathways of the second kind.