Deep Learning for Large-Scale Data-Driven Prediction of Electronic Properties

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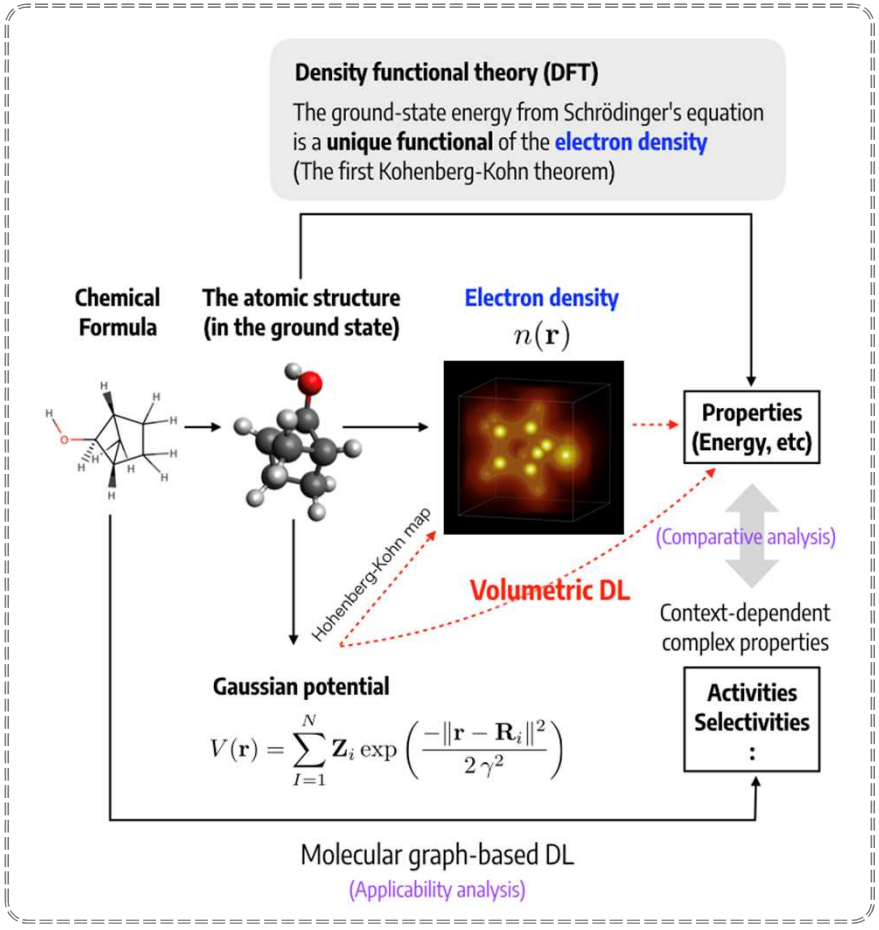
Research Area : Advanced Materials Informatics through Comprehensive Integration among Theoretical, Experimental, Computational and Data-Centric Sciences（PO：Shinji Tsuneyuki）

Brief overview

One of the most tedious, time-consuming, and error-prone step in materials informatics is the design and selection of descriptors, i.e. how to represent the targets in computers. We usually need to design different descriptors depending on whether the targets are isolated organic molecules, inorganic solid materials, or crystals. But from a machine-learning viewpoint, this situation resembles an early stage of the computer vision field where handcrafted descriptors are designed separately for hand-written characters, photos of faces, or photos of natural scenes. But thanks to the recent technical advances, these steps are significantly replaced by deep-learning based approaches. Similarly, the purpose of this research project is to investigate and evaluate the representation learning capability in material sciences powered by the state of the art deep learning and large-scale datasets.

Achievement

We established and evaluated data-driven prediction using volumetric deep learning based on *the 3D electron densities*. The first theorem of the Hohenberg-Kohn theorems, which is the foundation of the *density functional theory (DFT)*, states that there exists a one-to-one mapping between the ground-state wave function and the ground-state electron density. The ground-state electron density uniquely determines all properties, including the energy and wave function, of the ground state, and hence, they can be a promising candidate representations as universal descriptors of the molecules and materials. From more practical point of view, we also developed and evaluated the more direct 3D-3D volumetric learning (aka HK mappings) from an artificial volumetric potential to the electron densities.



Reference/Link

https://www.jst.go.jp/kisoken/presto/en/research_area/ongoing/areah27-4.html