Announcement of New Product Release : Advance/OF-DFT

Deep Learned Orbital Free-DFT

Kohn-Sham DFT (KS-DFT) has long been the standard method in density functional theory (DFT). However, KS-DFT is computationally expensive and challenging for simulating large systems due to its reliance on orbital (wave function) representation. Orbital Free-DFT (OF-DFT), which directly optimizes electron density without using orbitals, offers extremely fast simulations at a much lower computational cost. The main challenge with OF-DFT has been the lack of a practical kinetic energy functional.**AdvanceSoft Corporation has addressed this issue by applying its proprietary field deepening algorithm. We now offer services using our new product, Advance/OF-DFT, which incorporates the deep-learned kinetic energy functional AdvanceSoft25.**

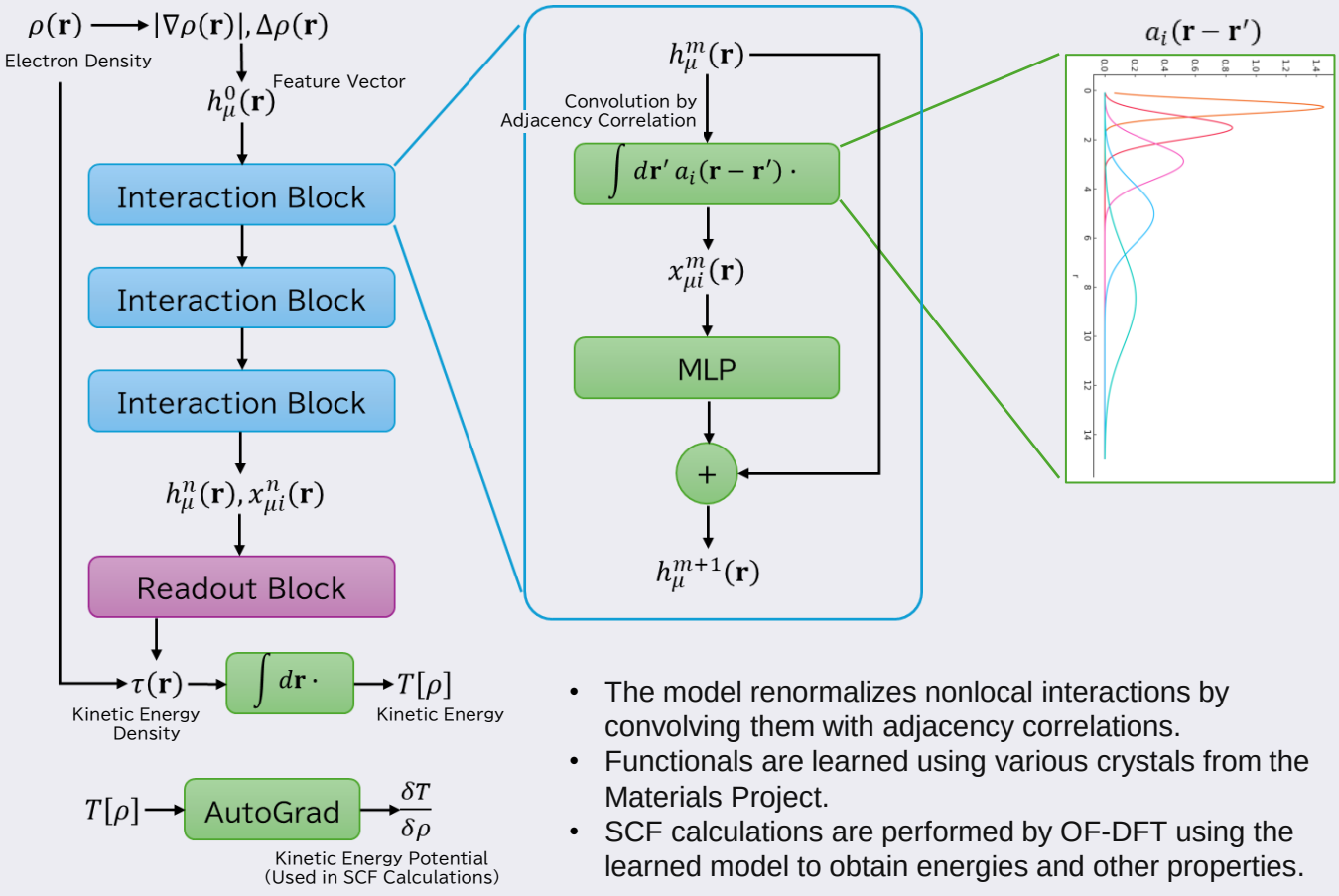
Kohn Sham-DFT vs Orbital Free-DFT

	KS-DFT	OF-DFT	Force Field
Electron Density	available	available	not available
Orbital (Wave Variables)	available	not available	not available
Kinetic Energy	Explicitly calculated in orbital	Deep Learned Functional : AdvanceSoft25	-
Calculation Accuracy	High	Depends on the functional	Depends on the force field
Calculation Cost	$O(N^3)$	$O(N)$	$O(N)$
Versatility	Applicable to all elements	Pseudo-potentials should be expanded (to be resolved in next version)	Ensure versatility with GNNP

Analyzing electronic structure, but same speed as GNNP

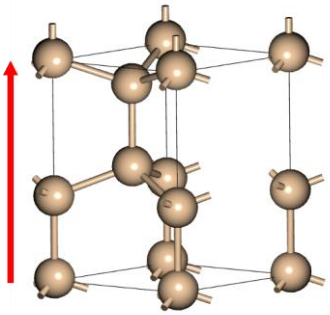
- The computational cost of OF-DF is proportional to the number of atoms (N), denoted as ($O(N)$), so simulations can be performed at the same level of computational speed as Graph Neural Network Potential (GNNP).
- Since information on electron density is retained, Bader charge can also be analyzed after convergence of the SCF calculation.
- Doping of electrons and holes is possible, and in combination with the Effective Screening Medium (ESM), large-scale MD simulations with controlled electrode potentials can be realized (ESM is not implemented in the current version). Application of an external electric field is also easy.
- The type of exchange-correlation functional can be selected at the time of SCF calculation, so non-local correlations corresponding to dispersion forces such as vdW-DF and rVV can also be used depending on the system; empirical functions such as DFT-D3 are not required.
- Since the wavefunction information is not included, a separate KS-DFT calculation is required for band structure and density of states calculations.

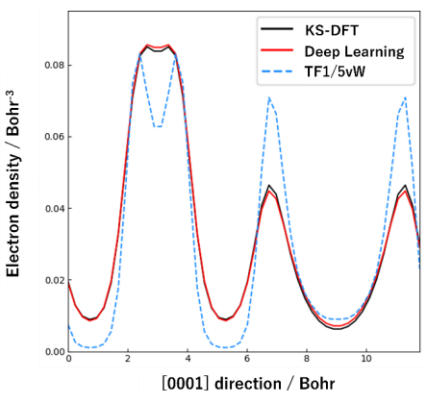
Architecture of the deep learned kinetic energy functional: AdvanceSoft25



- The model renormalizes nonlocal interactions by convolving them with adjacency correlations.
- Functionals are learned using various crystals from the Materials Project.
- SCF calculations are performed by OF-DFT using the learned model to obtain energies and other properties.

Electron density of hexagonal Si





If you are interested, please contact us. Benchmark calculations and other services are also available.

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