A Machine-Learning Surrogate Model for \textit{ab initio} Electronic Correlations

**Abstract**

The electronic structure in matter under extreme conditions is a challenging complex system prevalent in astrophysical objects and highly relevant for technological applications [1]. We show how machine-learning surrogates [2] in terms of neural networks have a profound impact on the efficient modeling of matter under extreme conditions. Our surrogate model that is trained on \textit{ab initio} quantum Monte Carlo (QMC) data can directly be used for various applications in the emerging field of warm dense matter research and beyond:

- **Diagnostics**: Interpretation of X-ray Thomson scattering experiments
- Nonlinear electronic density response
- Computation of material properties like thermal/electrical conductivity
- Electronic friction properties like the stopping power
- Advanced exchange-correlation functionals for density functional theory (DFT)
- Inclusion of electronic correlations in quantum fluid theories

**Warm Dense Matter (WDM)**

An extreme state with high temperature $T$ and density $n$.

- Astrophysical objects (giant planet / brown dwarf interiors, neutron star crusts, white dwarf envelopes, meteor impacts, ...)
- ICF: Inertial confinement fusion
- XFEL: Free electron lasers

**Electronic Density Response**

\[ G(q) = 1 - \frac{q^2}{4\pi} \left( \frac{1}{\chi_0(q)} - \frac{1}{\chi(q)} \right) \]

\( \chi(q) \): density response of actual electronic system, obtained from exact and computationally expensive QMC simulations, which are too costly for practical applications

\( \chi_0(q) \): density response of ideal (noninteracting) system

\( G(q) \): response of the system fully described by electronic local field correction $G(q)$

- **Goal**: Machine-learning representation of $G(q;r_s,\theta)$ covering the entire relevant parameter range [2]

- **Solution**: Fully connected deep neural network as universal function approximator combining input from different methods at different parameters

  - fast and accurate LFCs for practical applications

**Applications**

- **Example**: Interpretation of X-ray Thomson scattering experiments [3]

Our surrogate model (red, “ESA”), taken from Ref. [3] yields an accurate prediction of the scattering signal measured in aluminum (solid black, Ref. [4]). The computationally expensive TDFT curve performs substantially worse.

- This facilitates on-the-fly interpretation of experiments!

**References**


The surrogate model (dotted red) is even capable of predicting the nonlinear electronic density response (green points) of WDM, Ref. [5]