A Machine-Learning Surrogate Model for *ab initio* Electronic Correlations

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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 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:

- <u>**Diagnostics:**</u> 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

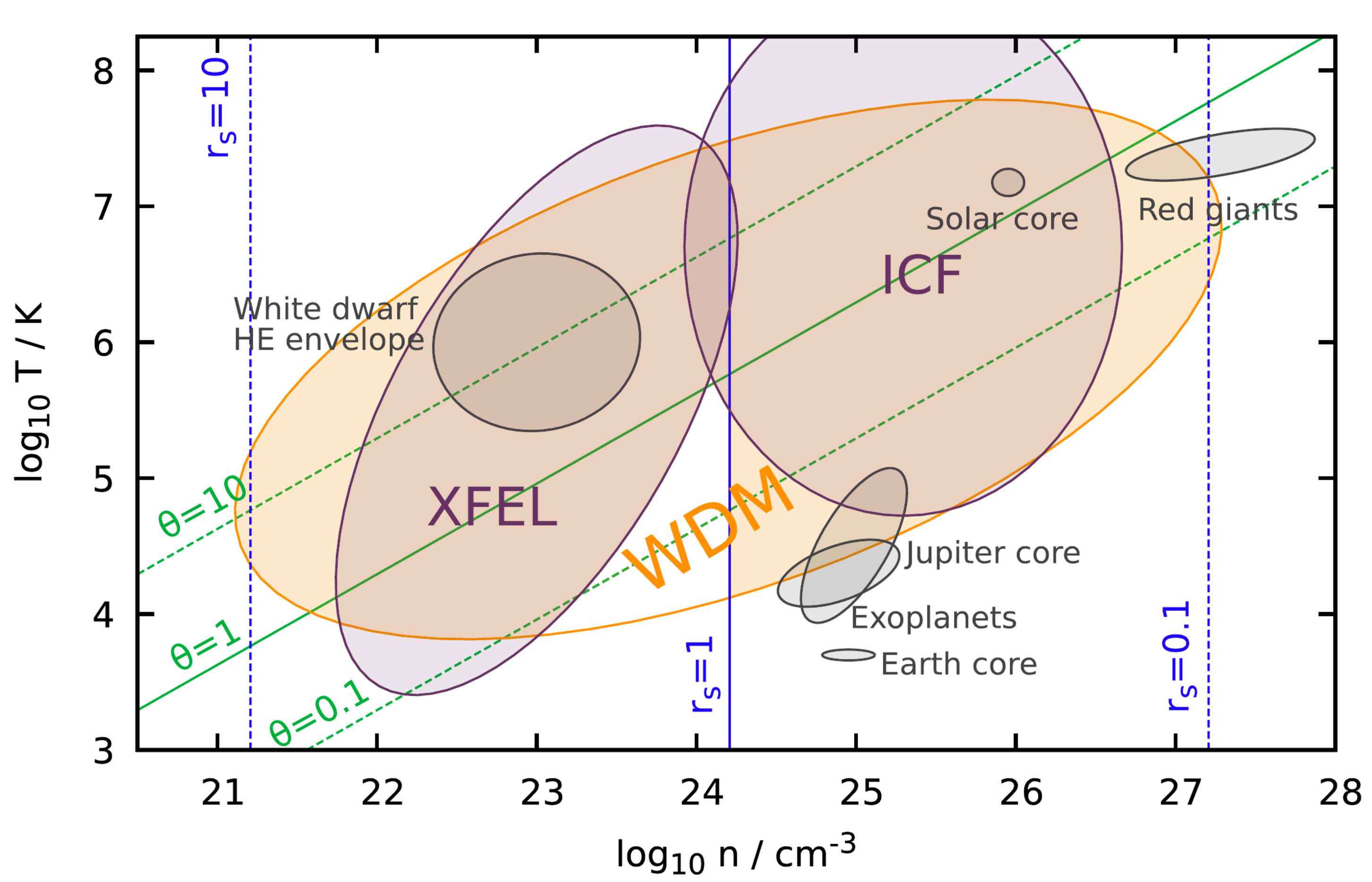
Warm Dense Matter (WDM)

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



Density-temperature plain with relevant physical examples. Taken from Ref. [1].

Electronic Density Response

→ Perturb a system at density parameter rs and temperature θ with wave-number q

→ <u>Linear response theory (LRT):</u> Response of the system fully described by **electronic local field correction** G(q)

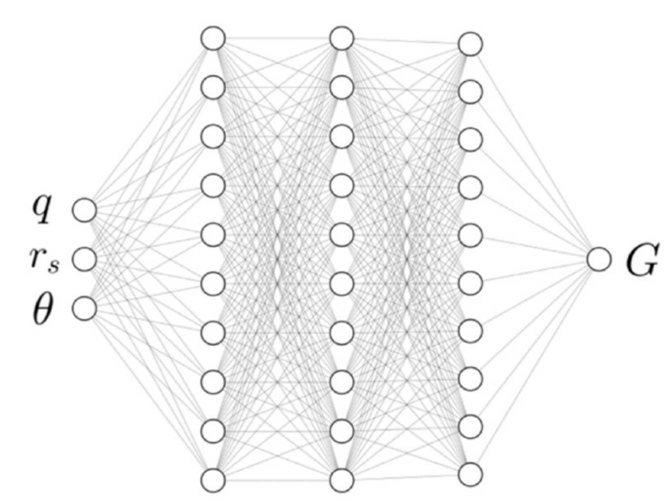
$$G(q) = 1 - \frac{q^2}{4\pi}\left(\frac{1}{\chi_0(q)} - \frac{1}{\chi(q)}\right)$$

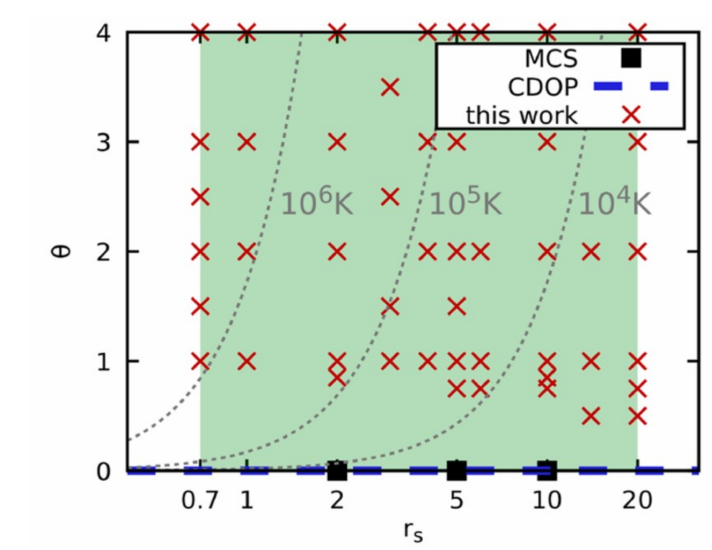
$\chi_0(q)$: density response of ideal (noninteracting) system

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

→ LFC is a measure for exchange correlation effects

Neural Network Representation of the LFC

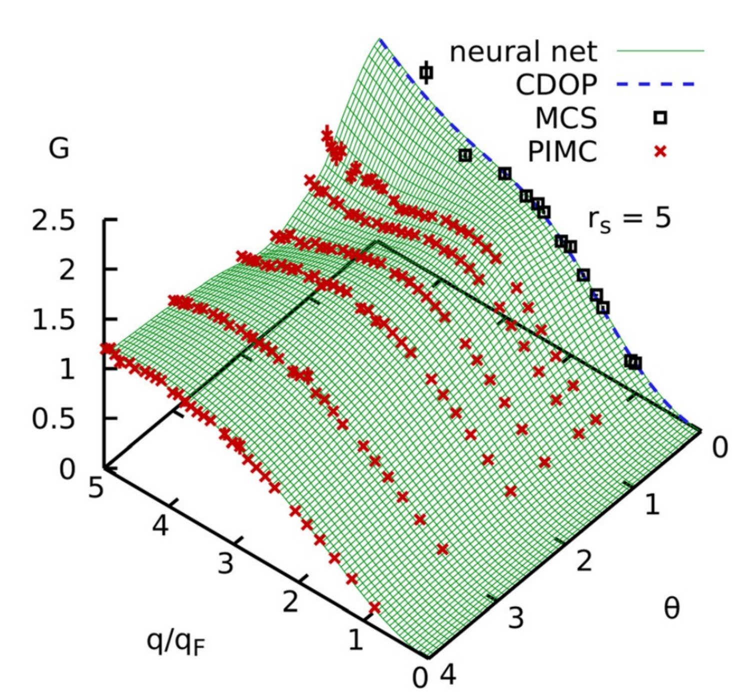




<u>**Goal:**</u> Machine-learning representation of G(q;rs,θ) covering the entire relevant parameter range [2]

<u>**Solution:**</u> Fully connected deep neural network as universal function approximator combining input from different methods at different parameters

→ **fast and accurate LFCs** for practical applications



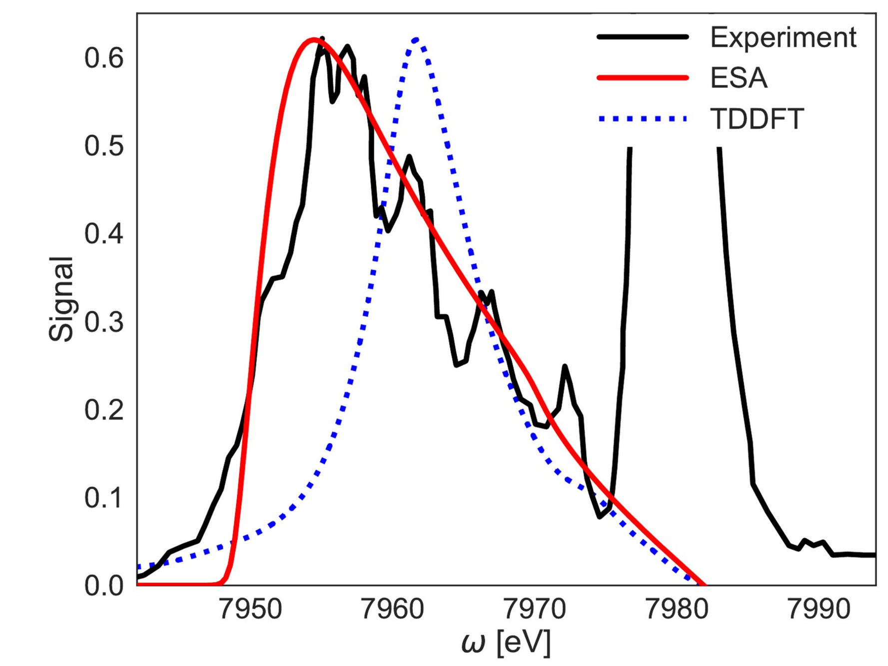
<u>**Machine-learning representation of the electronic local fied correction**</u>

Green surface: prediction of neural network
Red crosses: QMC data at finite T
Black squares: QMC data at T=0

Taken from Ref. [2]

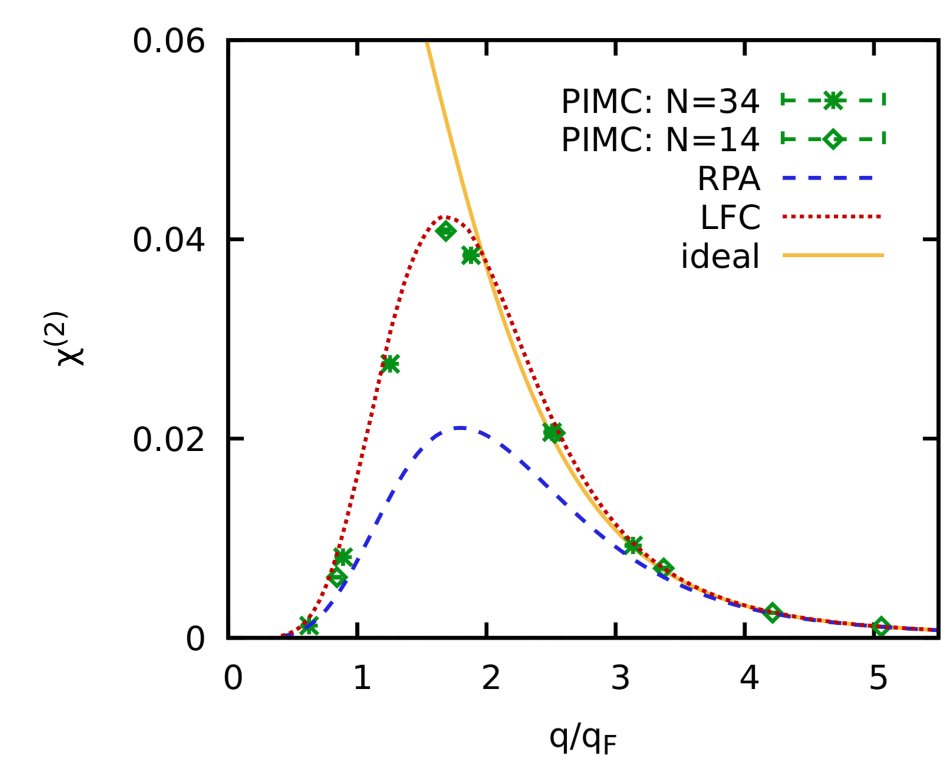
Applications

<u>Example:</u> 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 TDDFT curve performs substantially worse.

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



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

References

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[2] T. Dornheim et al. (2019). "The static local field correction of the warm dense electron gas". In: J. Chem. Phys. **151**, pp. 194104

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[5] T. Dornheim et al. (2021). "Density Response of the Warm Dense Electron Gas beyond LRT: Excitation of Harmonics". In: arxiv:2104.02405