Materials Learning Algorithms (MALA): Learning the electronic structure of materials with neural networks

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CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

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HZDR HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF
TECHNISCHE UNIVERSITÄT DRESDEN
CBG Max Planck Institute of Molecular Cell Biology and Genetics
HELMHOLTZ CENTRE FOR ENVIRONMENTAL RESEARCH – UFZ
Uniwersytet Wrocławski

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Multiscale modeling of materials under extreme conditions

- Modeling of materials under extreme conditions across several length and time scales

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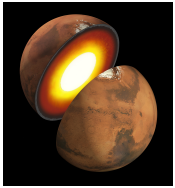
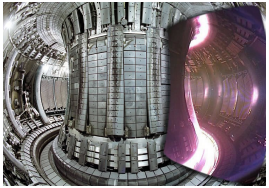
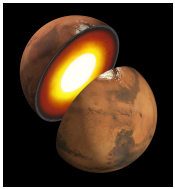
- Important for advanced applications (astrophysics, materials discovery, …)

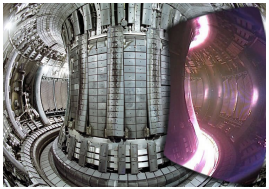


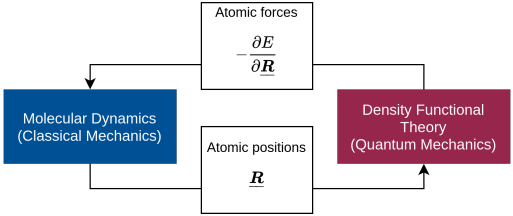


Multiscale modeling of materials under extreme conditions

- Modeling of materials under extreme conditions across several length and time scales
- Important for advanced applications (astrophysics, materials discovery, …)
- Combination of multiple simulation methods required







FT-DFT and surrogates

- Simulations via KS-DFT at $\tau > 0K$, approximating grand canonical ensemble

$$\left[-\frac{1}{2}\nabla^2 + v_{\mathrm{s}}^{\tau}(\boldsymbol{r})\right]\phi_j(\boldsymbol{r}) = \epsilon_j^{\tau}\phi_j(\boldsymbol{r}) \,, \tag{1}$$

$$n(\boldsymbol{r}) = \sum_j f^{\tau}(\epsilon_j^{\tau})\,|\phi_j(\boldsymbol{r})|^2 \,, \tag{2}$$

$$A_{\mathrm{total}}^{\mathrm{BO}}[n] = T_{\mathrm{s}}[\phi_j] - \tau S_{\mathrm{s}}[\phi_j] + E_{\mathrm{H}}[n] + E_{\mathrm{xc}}^{\tau}[n] + E^{ei}[n] + E^{ii} \,, \tag{3}$$

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  - High temperature require large number of KS wave functions

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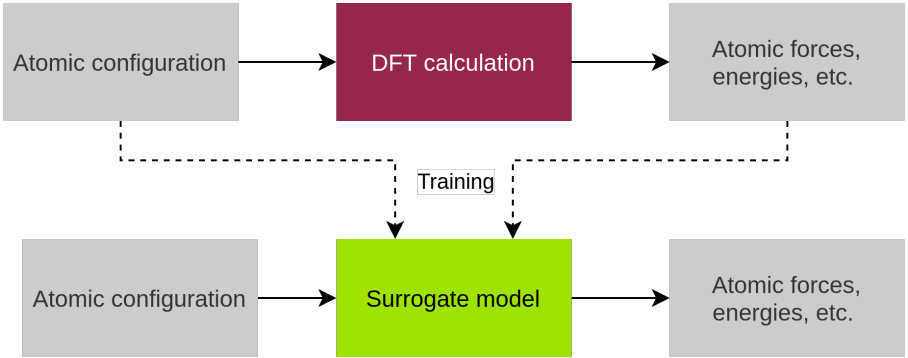

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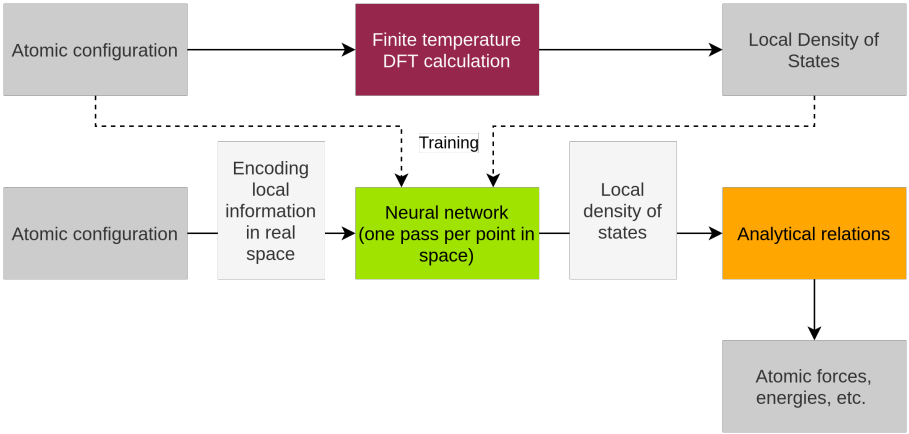
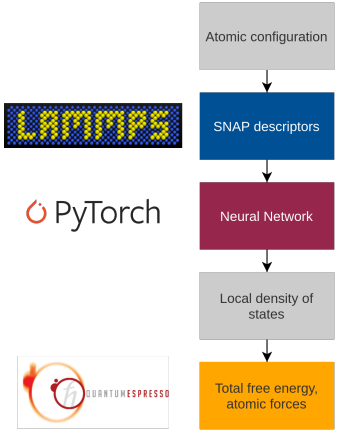


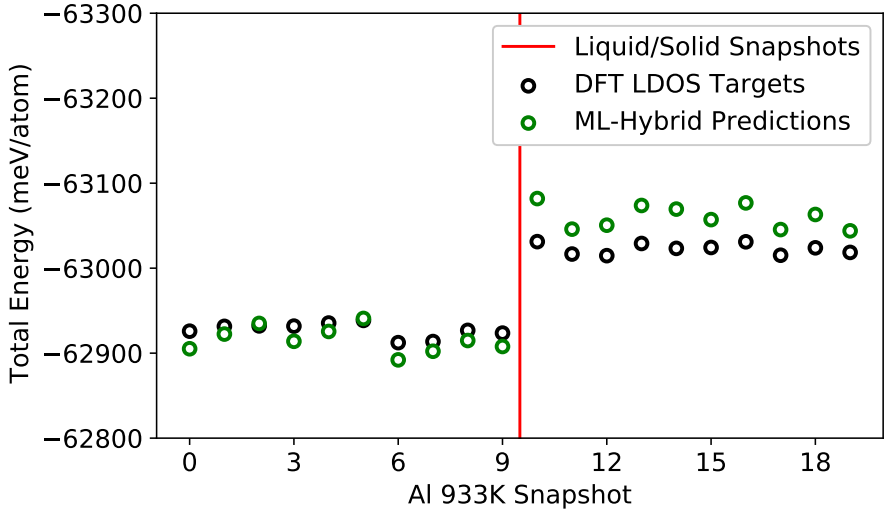
Framework for learning LDOS: MALA



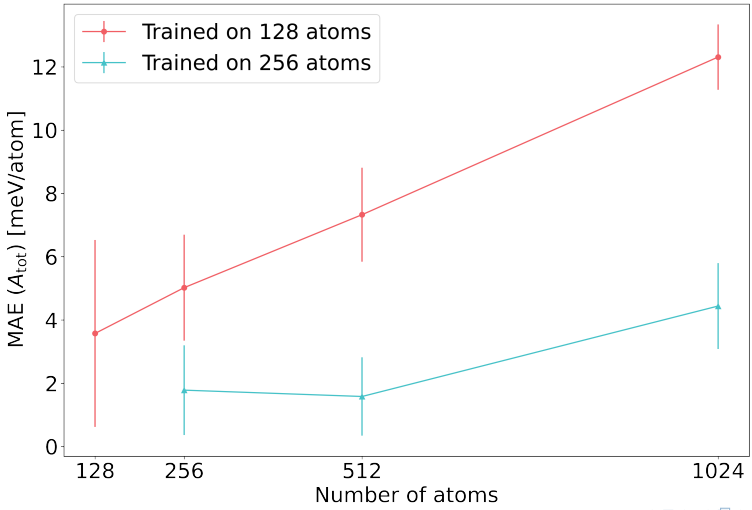
- Encoding of local information using SNAP descriptors (LAMMPS code)
- Feed-foward neural networks built and trained using PyTorch
- Local Density of States post-processed using analytical relations and QuantumESPRESSO
- Data generation done via VASP (DFT-MD) and QE (DFT, DFT-MD)

Materials Learning Algorithms

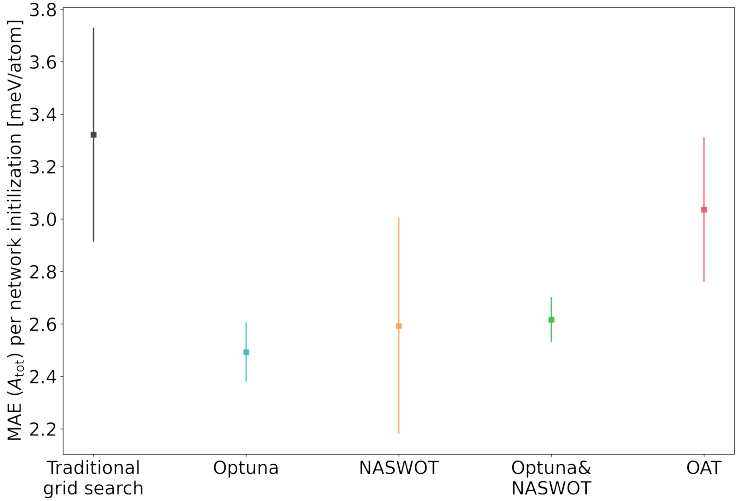
Results I: Proof of concept (Aluminium at 933K)



Results II: Size transfer (Beryllium at 298K)



Results III: Hyperparameter optimization (Aluminium at 298K)



Conclusion / Outlook

- Accurate surrogate models can be created based on LDOS

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- Accurate surrogate models can be created based on LDOS
- Size transfer between models possible if training data is carefully selected
- Application to larger temperatures
- Calculation of physical quantities of interest via MD or Monte-Carlo

MALA cooperation partners

Check MALA out on GitHub: https://github.com/mala-project

J. A. Ellis, L. Fiedler, G. A. Popoola, N. A. Modine, J. A. Stephens, A. P. Thompson, A. Cangi, and S. Rajamanickam.
Accelerating finite-temperature kohn-sham density functional theory with deep neural networks.
Phys. Rev. B, 104:035120, Jul 2021.

Thank you for your attention!

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