Demonstrating temperature transferability of neural network models replacing modern density functional theory

35th Electronic Structure Workshop

14.06. // Lenz Fiedler, Attila Cangi

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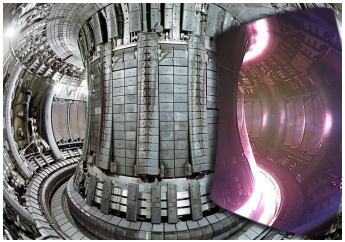
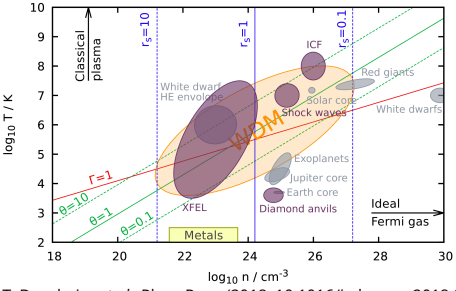
Motivation: Modeling of materials under extreme conditions

- Large scale simulations at ambient conditions and towards the warm dense matter regime (temperatures of $10^4 - 10^8$K)





T. Dornheim *et al.*, Phys. Rep., (2018, 10.1016/j.physrep.2018.04.001)

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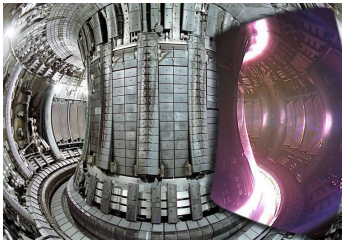

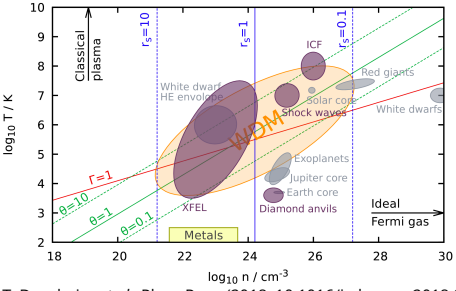

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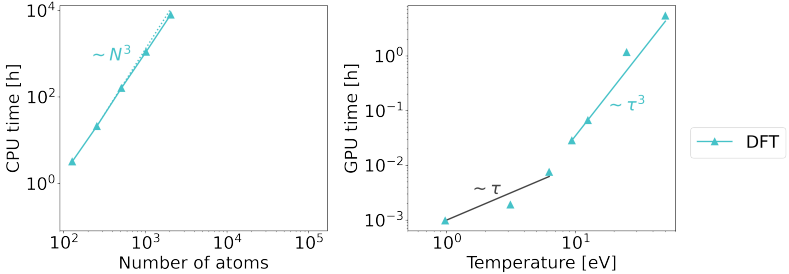

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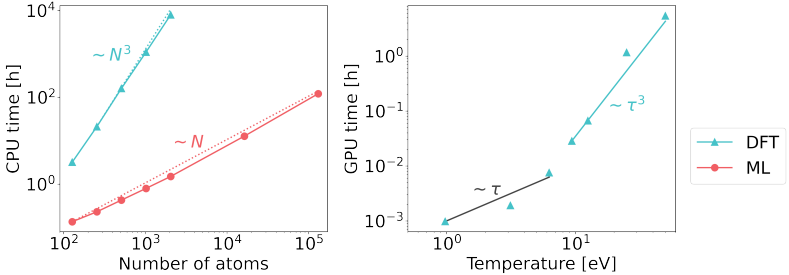
- Possible solution: models that directly learn electronic structure



L. Fiedler *et al.*, accepted in npj Comput. Mater. (10.48550/arXiv.2210.11343)

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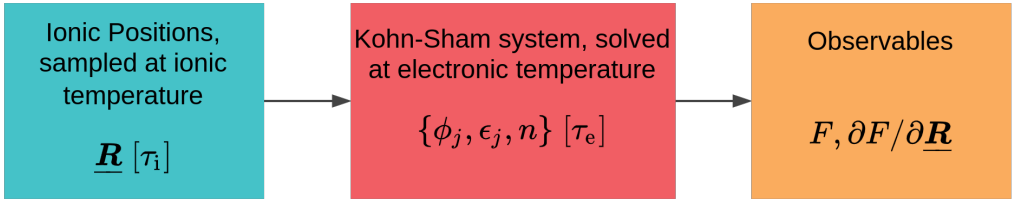

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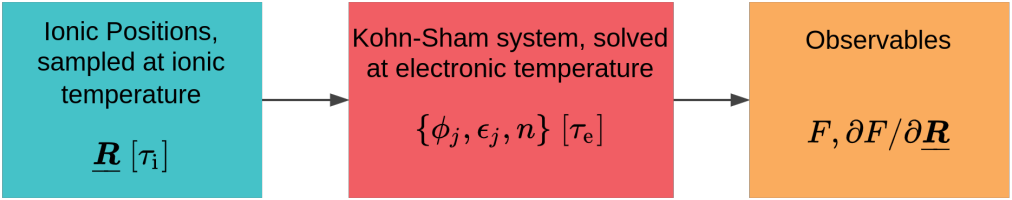

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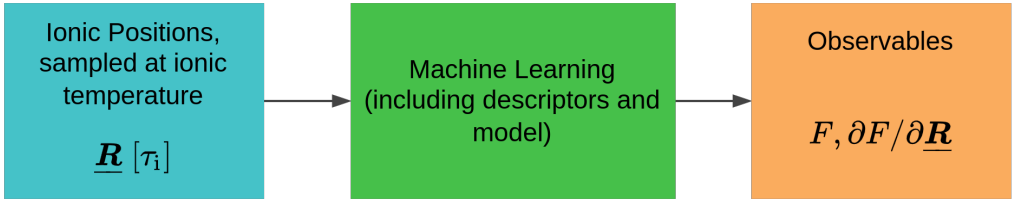
- Models usually do not take τ_e into account



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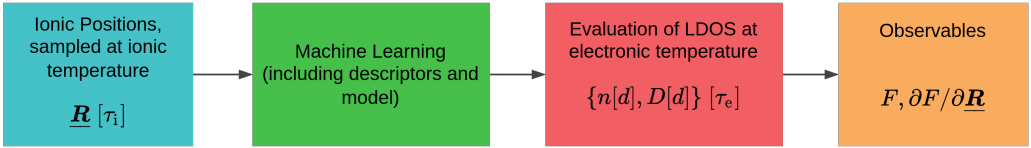

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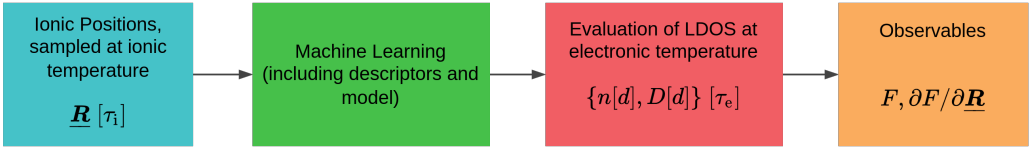

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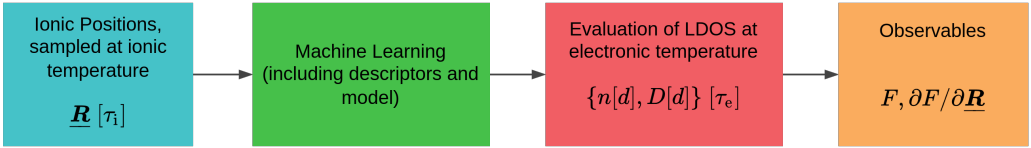

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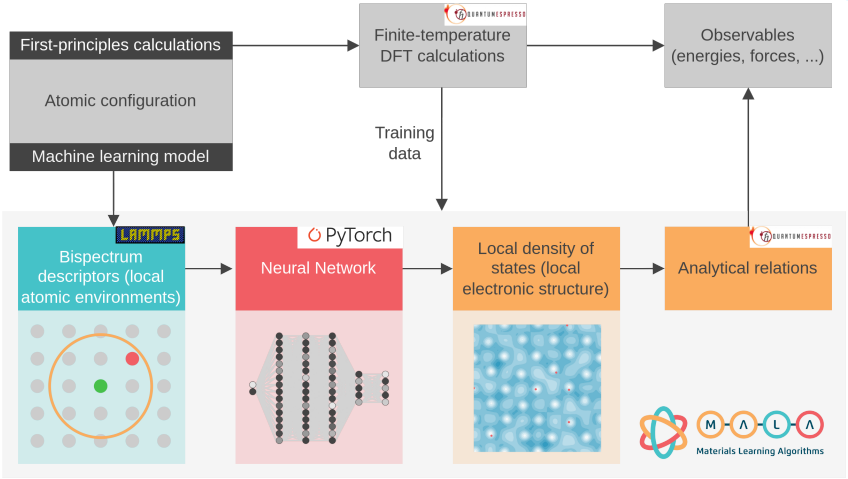

J.A. Ellis *et al.*, Phys. Rev. B (2021, 10.1103/PhysRevB.104.035120)

L. Fiedler *et al.*, Mach. Learn.: Sci. Technol. (2022, 10.1088/2632-2153/ac9956)

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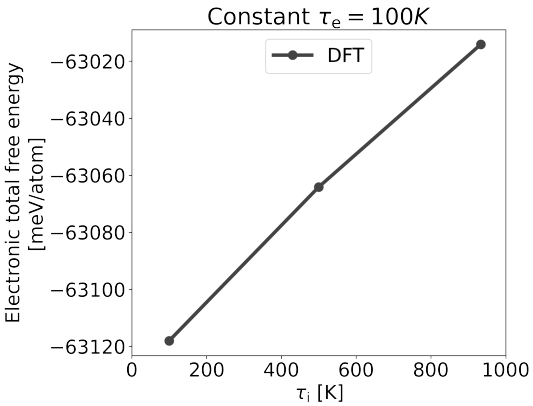

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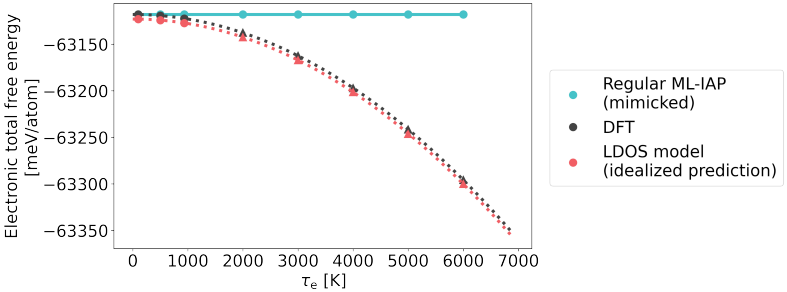

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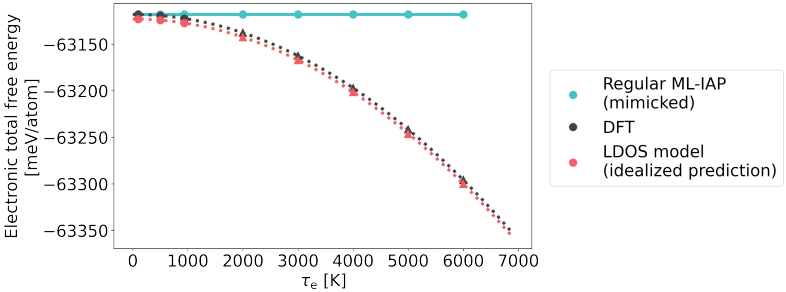

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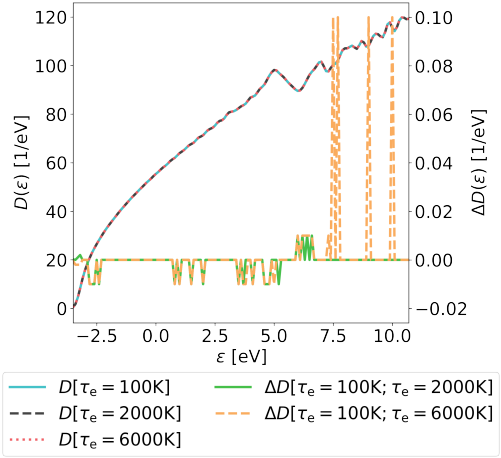

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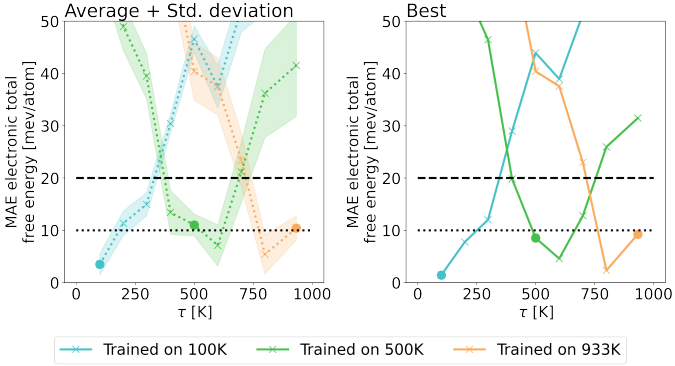

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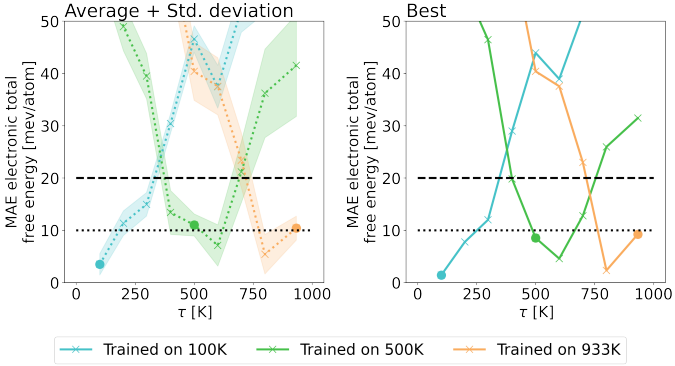
- Models in principle capable of temperature transfer, but multiple data points necessary



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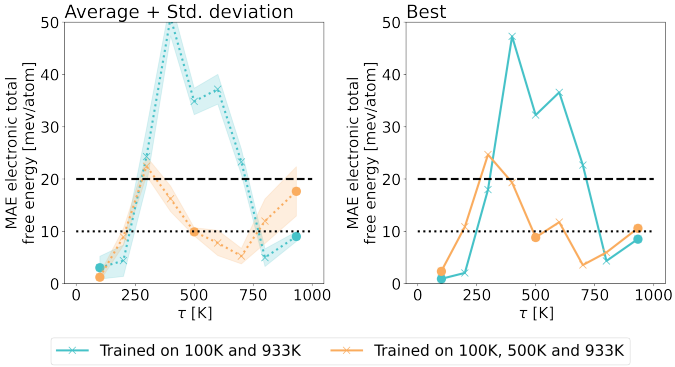

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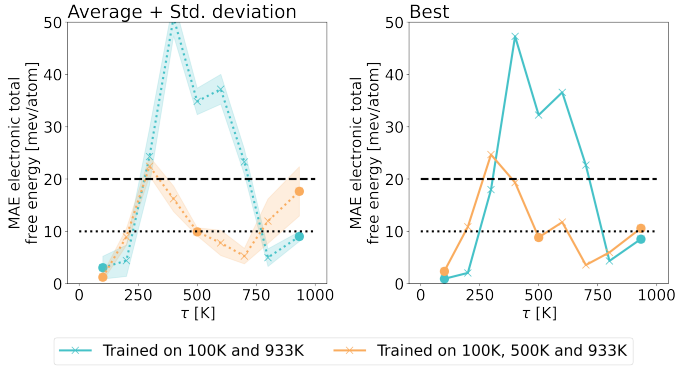

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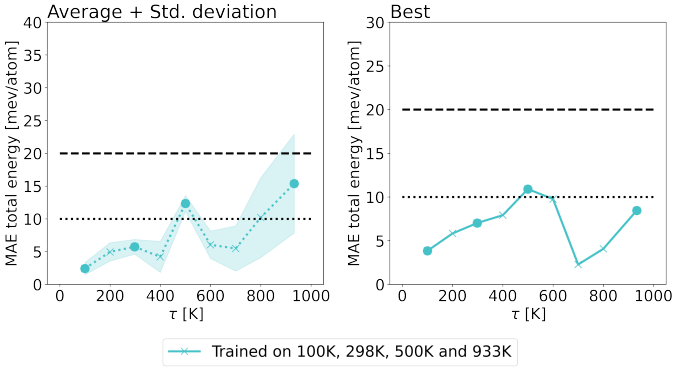
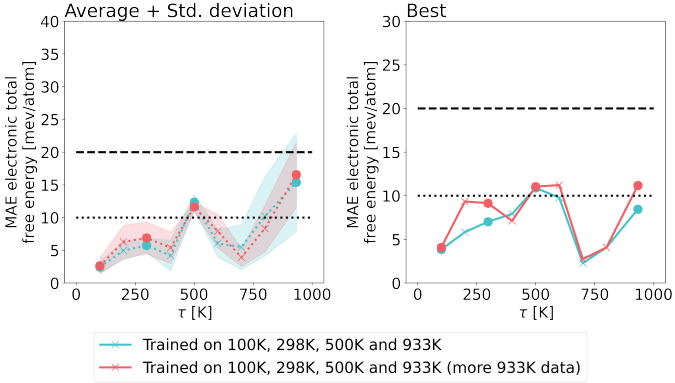


Temperature transfer with MALA models

- More data at 933K needed



Temperature transfer with MALA models

- Extrapolation with models in the τ_e domain becomes possible

Temperature transfer with MALA models

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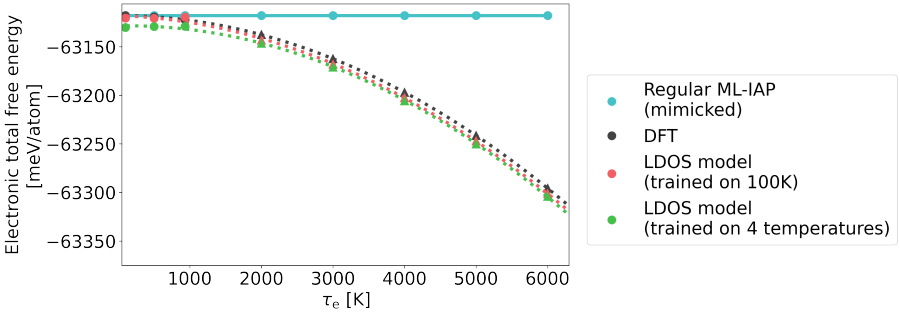
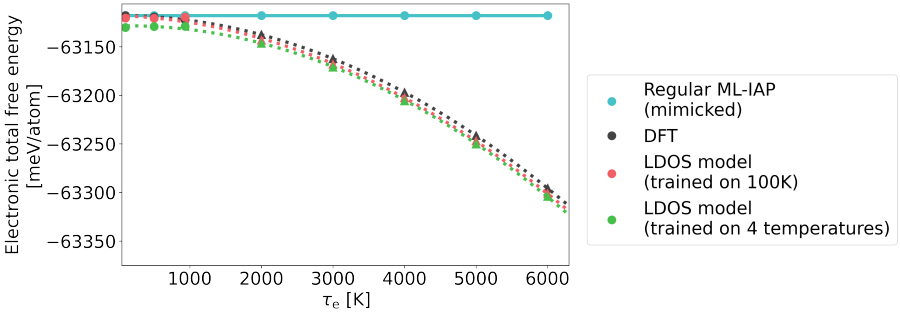


Temperature transfer with MALA models

- Extrapolation with models in the τ_e domain becomes possible
- E.g. for laser heated electrons



MALA cooperation partners

Sandia National Laboratories

Normand A. Modine, Kyle D. Miller

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

Thank you for your attention!

Further Reading: L. Fiedler, N.A. Modine, K.D. Miller, A. Cangi:
Machine learning the electronic structure of matter across temperatures,
10.48550/arXiv.2306.06032

Computational details

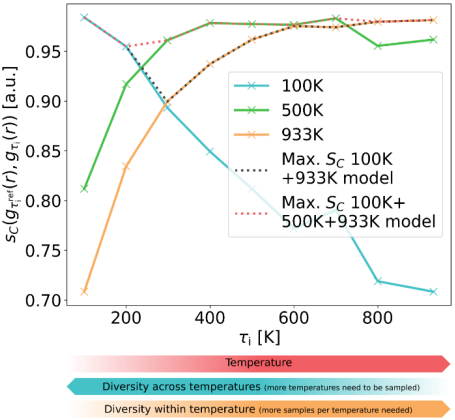
Parameter	Aluminium
Number of atoms	256
PW cutoff	100 Ry
$\boldsymbol{k}$-grid	$8 \times 8 \times 8$
XC functional	PBEsol
Pseudopotential	Scalar-relativistic, optimized norm-conserving Vanderbilt
Temperatures	100K, 200K, 298K, 400K, 500K, 600K, 700K, 800K, 933K

Computational details

Parameter	2 temperatures	3 temperatures	4 temperatures
Network size		$91 \times 4000 \times 4000 \times 4000 \times 250$	
Learning rate		0.00005	
Activation function		LeakyReLU	
Optimizer		Adam	
Training data set	$4 \times 100K$ $4 \times 933K$	$4 \times 100K$ $4 \times 500K$ $4 \times 933K$	$4 \times 100K$ $4 \times 298K$ $4 \times 500K$ $4 \times 933K$

Temperature transfer with MALA models

- Analysis via cosine similarity S_C reveals larger structural differences at smaller temperatures



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