# Data-driven Surrogate Modeling of Matter under Extreme Conditions with the Materials Learning Algorithms Package (MALA)

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## Motivation

Accurate numerical modeling of extreme states of matter (warm dense matter) requires multiscale materials modeling across length and time scales near first-principles accuracy.

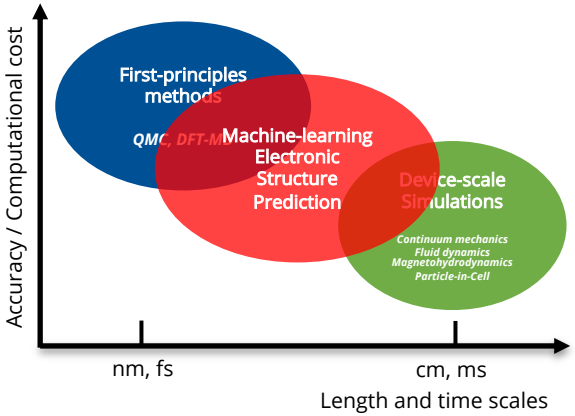
## Challenge

This requires data generation of electronic structures of diverse atomic configurations at a scale which is infeasible with current algorithms.

## Goal

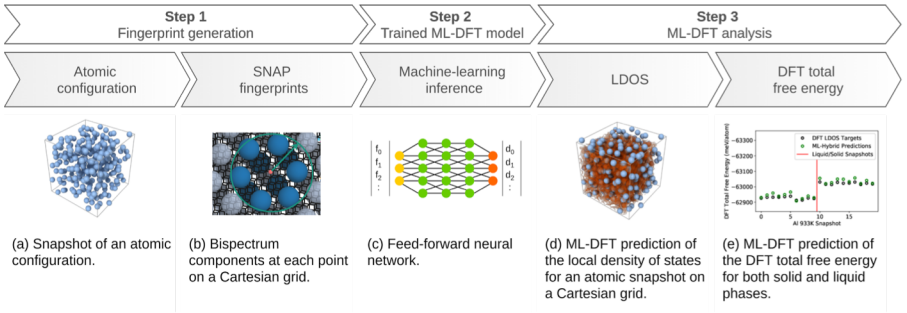
We bypass the computational bottleneck of DFT by leveraging machine learning to enable applications relevant for:

- Physics of planetary and stellar interiors
- ICF capsules on their pathway towards ignition
- Radiation damage in both fission and fusion reactor walls
- Novel materials discovery




## Methods and Results

Workflow of machine-learning surrogate model replacing traditional Kohn-Sham density functional theory calculations for materials at a given temperature and pressure.




(a) Snapshot of an atomic configuration.

(b) Bispectrum components at each point on a Cartesian grid.

(c) Feed-forward neural network.

(d) ML-DFT prediction of the local density of states for an atomic snapshot on a Cartesian grid.

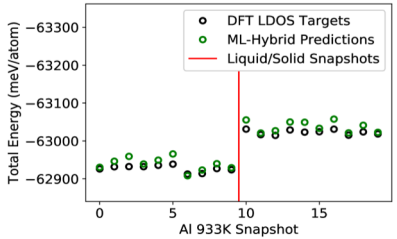
(e) ML-DFT prediction of the DFT total free energy for both solid and liquid phases.

## Key result

### Unified ML model for both liquid and solid aluminum

A single ML-DFT model yields accurate results (LDOS, electronic density, band energy, and total energy) for both crystalline and liquid aluminum.

Total (free) energies agree with conventional DFT calculations to well within chemical accuracy (1 kcal/mol = 43.4 meV/atom).




## Software development

Materials Learning Algorithms

https://github.com/casus/mala_poc

Open source software releases planned in stages along with key publications.

## Preprint

You can find further details in our preprint (arXiv:2010.04905).

For further questions please contact a.cangi@hzdr.de.

## Collaborators, Stakeholders, Press

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