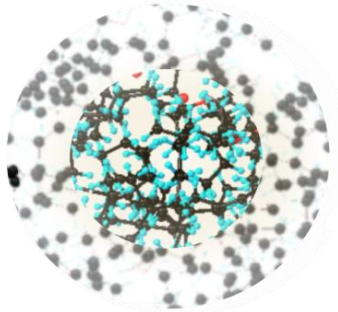
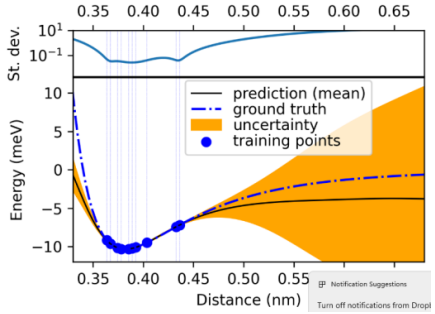
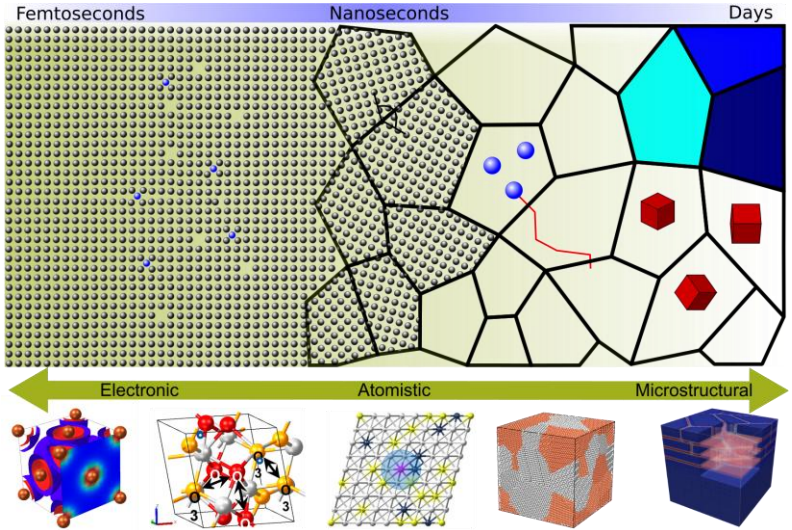
materials design





Machine and Human Learning of Materials



Leonid Kahle

Research Scientist, Materials Design S.A.R.L

17 Oct 2025

Human Learning of Materials

Human Learning Timeline

2010-2013	2013-2015	2015	2015-2019	2020-2021	2021-present
BSc (Materials Science) in Kiel	MSc in Materials Science, EPF Lausanne	Numerical simulations at Bosch Research, Cambridge (USA)	PhD at EPFL on simulations of battery materials (2015-2019)	PostDoc at IBM Research Zurich on NLP and deep-model uncertainty	Scientist at Materials Design S.A.R.L. (Montrouge)


Kiel (D)


EPF Lausanne (CH)


Cambridge (US)


IBM Zurich (CH)


Thun (CH)

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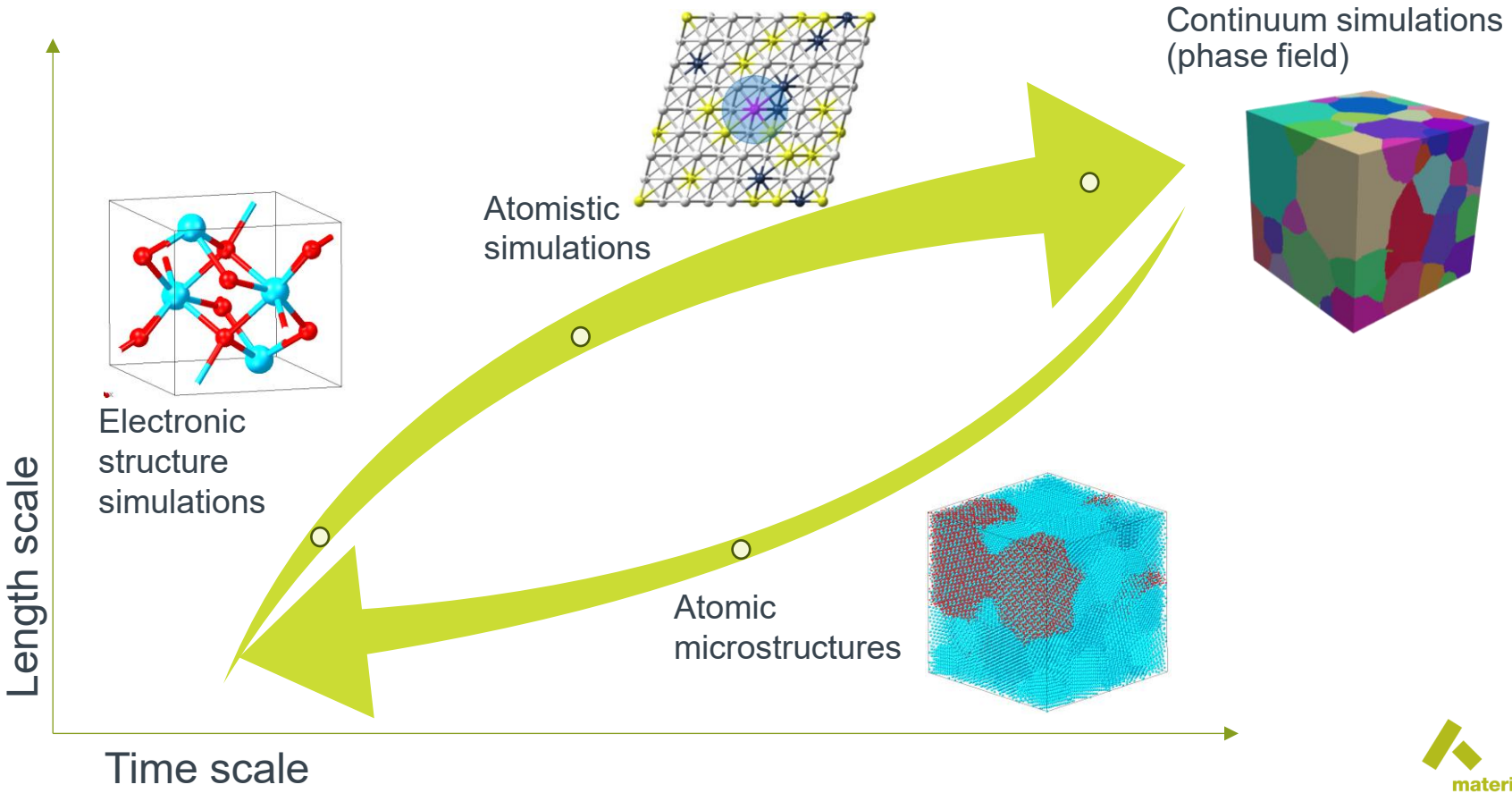
Accessing different time and length scales



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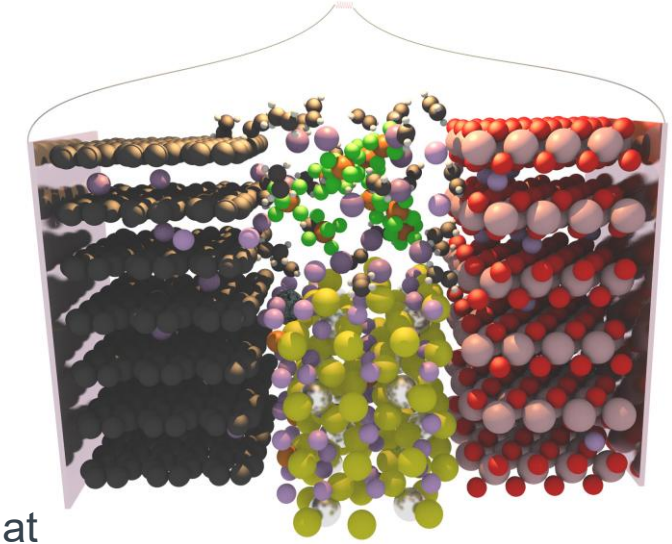
Machine Learning of Materials

Material Science at the atomic scale

Task: finding a better battery material!

How much Li fits into the anode?

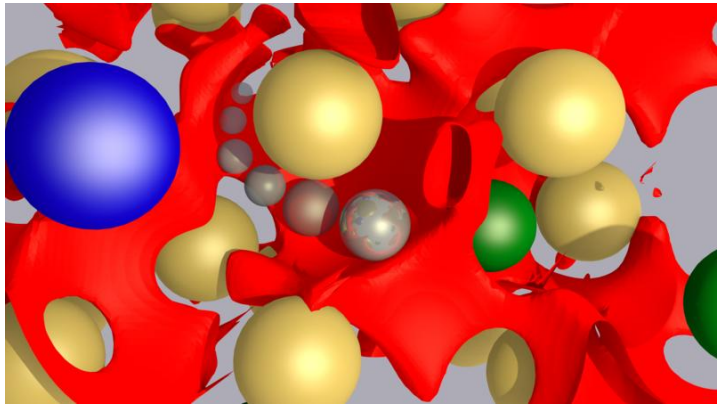


What is the voltage of an anode/cathode?

What are good materials for electrolytes with high electronic resistance and high ionic conductivity?

Which materials are stable at such voltages?

What is the ground truth?

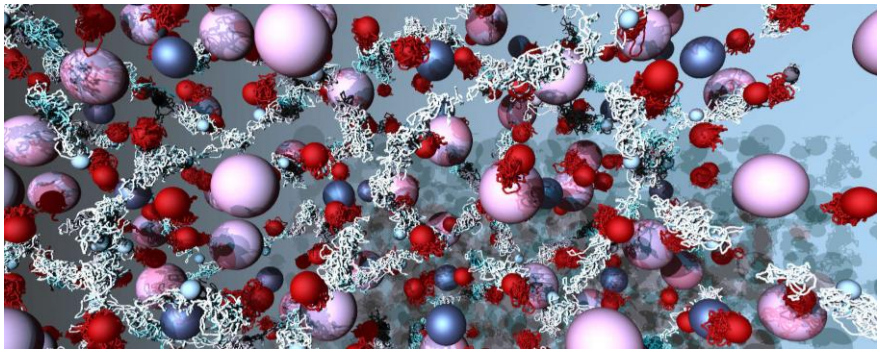


Electronic properties: $\hat{H}\Psi = E\,\Psi$

To calculate electronic properties from first principles, we need to solve (approximations to) the Schrödinger's equation.

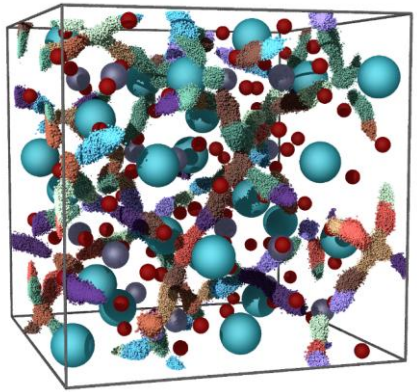
Dynamic properties: $F = ma$

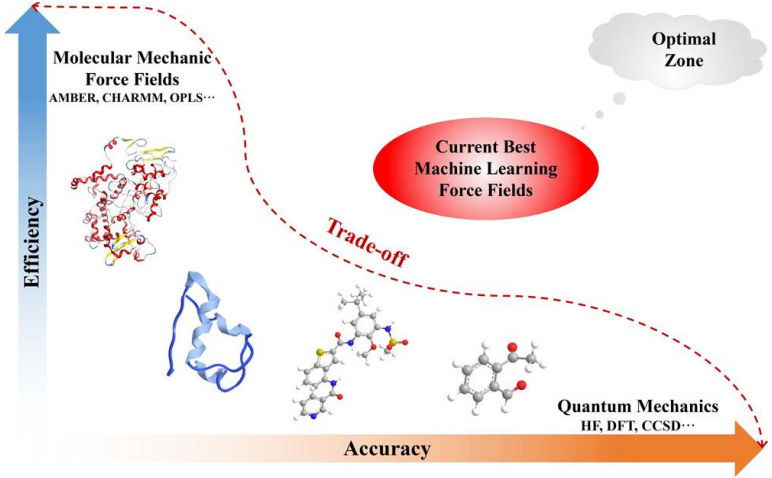
To calculate dynamic properties, we integrate the forces on atoms over time.



Machine learning in dynamic simulations

Machine learning can help analyze simulations with “classical” methods, e.g., using unsupervised learning of the atomic environment [1]

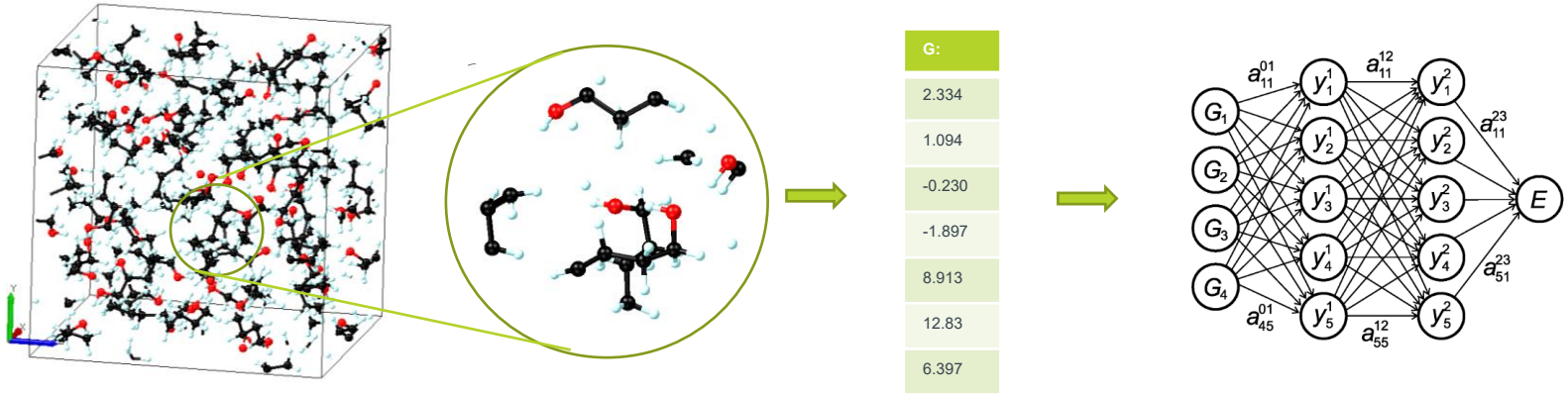




Machine learning interatomic potentials can drive dynamic simulation combining high accuracy of advanced QM methods at the cost of empirical potentials.

[1] Kahle et al., Unsupervised landmark analysis for jump detection in molecular dynamics simulations, Phys. Rev. Mat. 3, 055404 (2019)

Obtaining an Atomistic ML Potential for Organics



Challenge in organic liquids are the different contributions:

- Complex, strong, short-range covalent bonding.
- Simple, weaker, long-range vdW and electrostatic interactions.
- Very complex environments.

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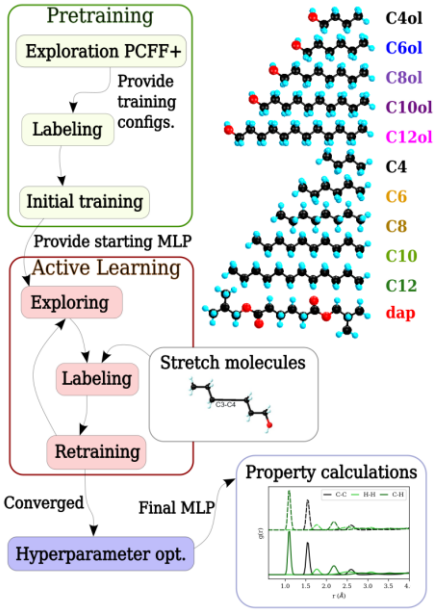
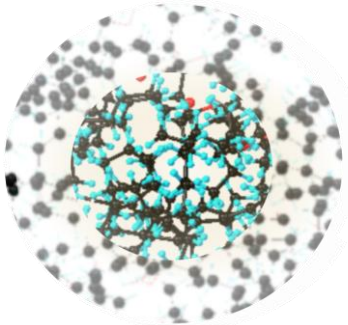
Learning about alcohol!

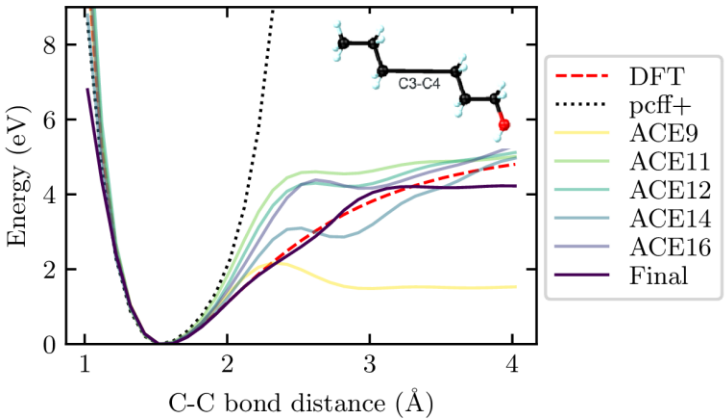


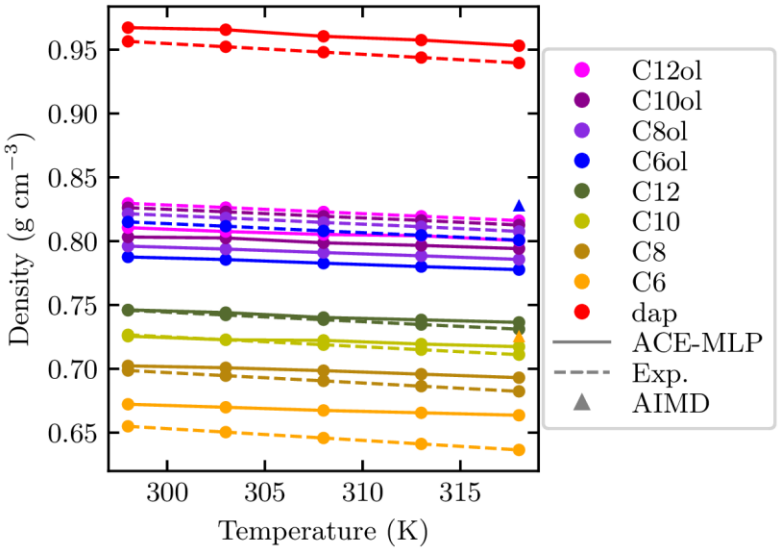
- An industry client wants to understand heat transfer between metals and alcohols
- No empirical model → Train a machine learning interatomic potential (MLIP)
- Complex short intramolecular and simple long-range intermolecular interactions -> A dual cutoff MLIP
- Active learning for training set generation.



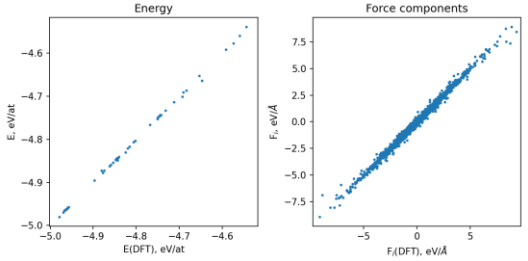
Kahle et al., A dual-cutoff machine-learned potential for condensed organic systems obtained via uncertainty-guided active learning, Phys. Chem. Chem. Phys., 2024, 26, 22665

Learning about alcohol!





- Subsequent iterations of active learning improve results.
- How to add training data is the key!
- Good final reproduction of density (not trained!)



Kahle et al., A dual-cutoff machine-learned potential for condensed organic systems obtained via uncertainty-guided active learning, Phys. Chem. Chem. Phys., 2024, 26, 22665

Predicting Uncertainty of Deep Models

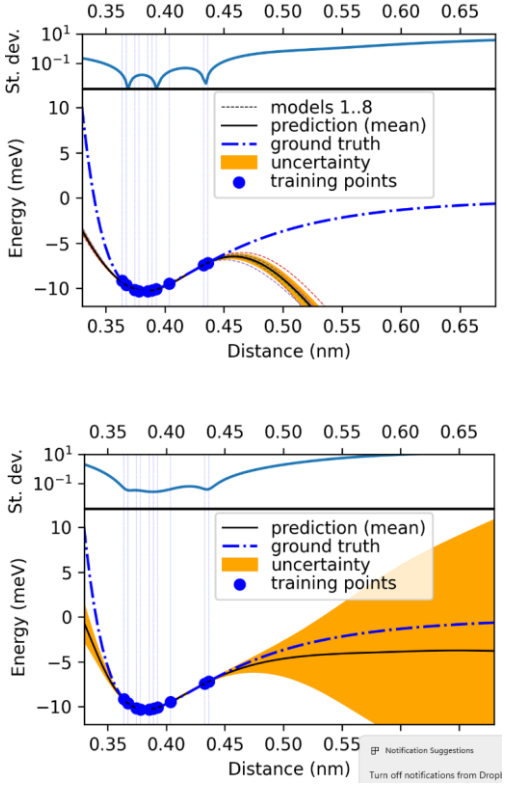
- ML predictors extrapolate badly (hallucinations)

Name 5 fruits with 2 times the letter R

Here are **5 fruits** that each contain the letter **R** twice:

1. Cherry
2. Currant
3. Blackberry
4. Raspberry
5. Strawberry

- The same can happen with MLIPs, *out-of-distribution* predictions will be wrong – and we don't know!
- How can we estimate deep NN uncertainty?



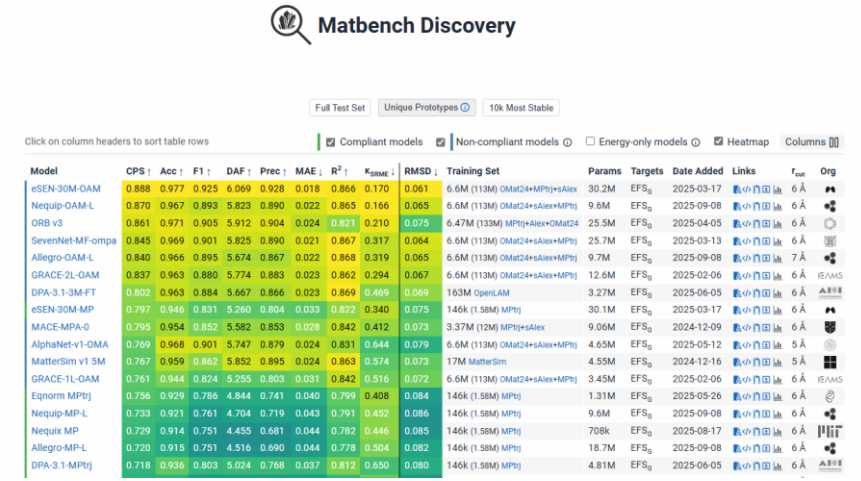
Kahle and Zipoli., Quality of uncertainty estimates from neural network potential ensembles, PRE 105, 015311 (2022)

Making predictions…

Trends and observations, predictions and hallucinations

Trends and observations:

- A new ML model every few months.
- Foundational MLIPs are coming.
- Do we have the right performance metrics ?
- Data quality & quantity is a challenge.



https://matbench-discovery.materialsproject.org/

3 predictions for ML in (materials) science:

- AI will not replace creative thinkers with domain knowledge.
- Understanding underlying theory (of ML and materials science) is key to progress.
- Bright future for machine-learning experts in materials science.