# Otaniemi Center for Atomic-scale Materials Modeling (OCAMM)
## Possibilities for academia and industry

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High-performance computing - Business cooperation
19 September 2023

**turbogap.fi** **miguelcaro.org**

Aalto University
School of Chemical
Engineering

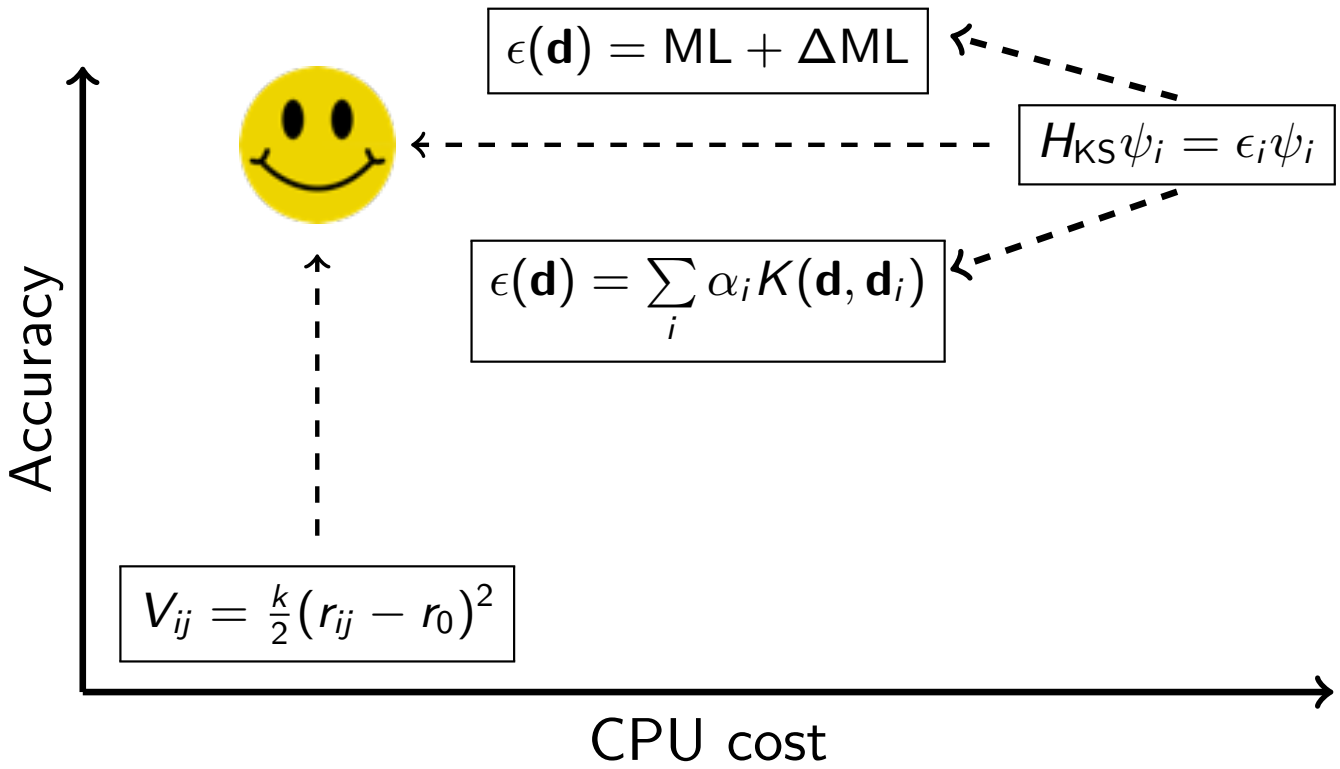
SUOMEN AKATEMIA
FINLANDS AKADEMI
ACADEMY OF FINLAND

CSC

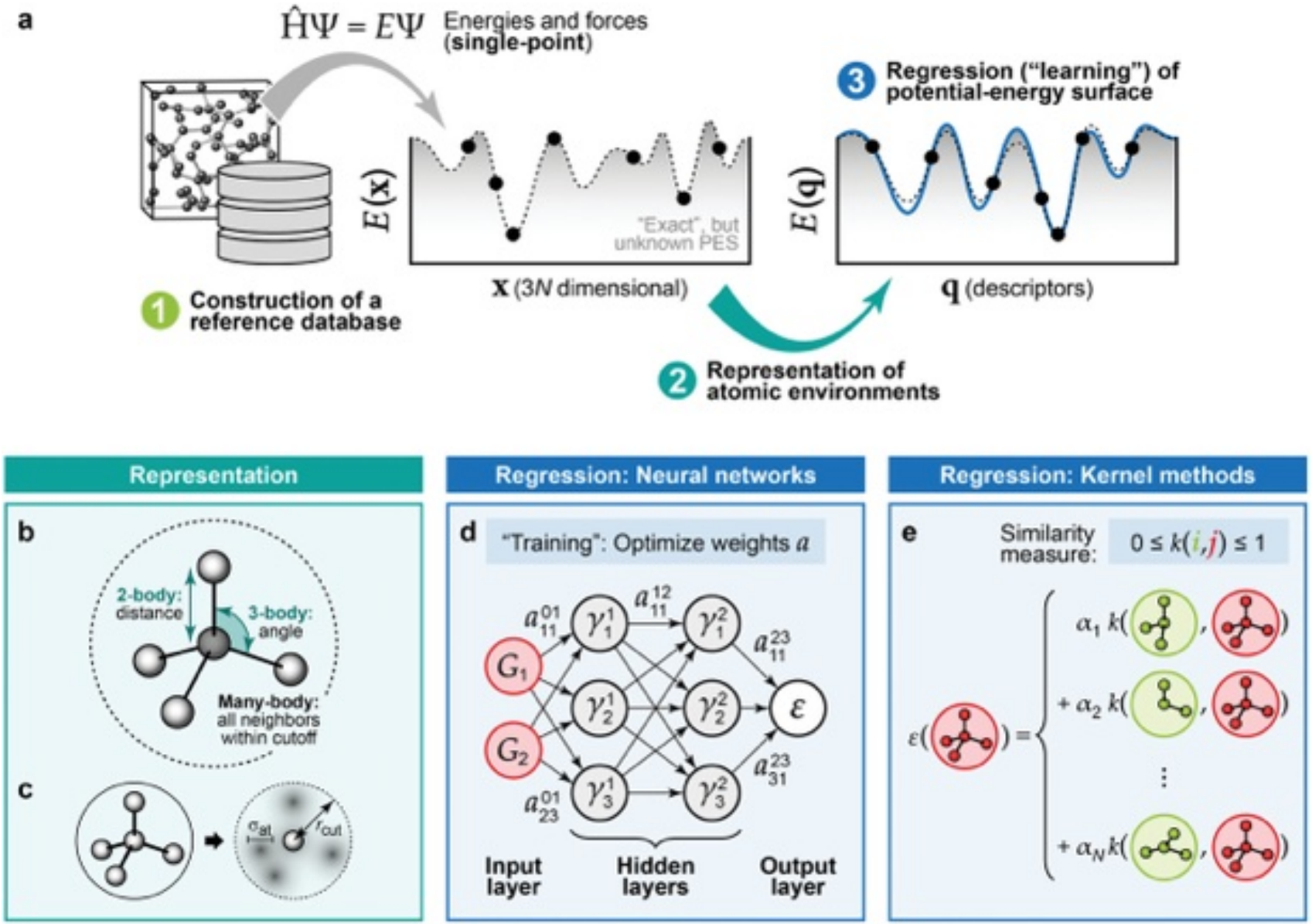
TurboGAP
Data-driven atomistic simulation

# The dream: computational experimentation

- Quantum mechanical description of atomic interactions is very expensive
- "Classical" interatomic potentials are not accurate enough
- With machine-learning potentials we can improve (some) things!
- In some cases we can "fix" issues with DFT (usually ΔML)



# AI-driven "golden age" in atomistic materials modeling




**Adv. Mater. 31, 1902765 (2019)**

# Why do we need to make realistic predictions?

- Accurate models for **reliability**: learn from quantum-mechanics
- "Cheap" models: AI algorithms speed up calculations (a lot!)
- Cheap + accurate = more atoms and longer simulations = more realistic
- Implemented in efficient codes and powerful supercomputers

**expectation**

**vs**

reality

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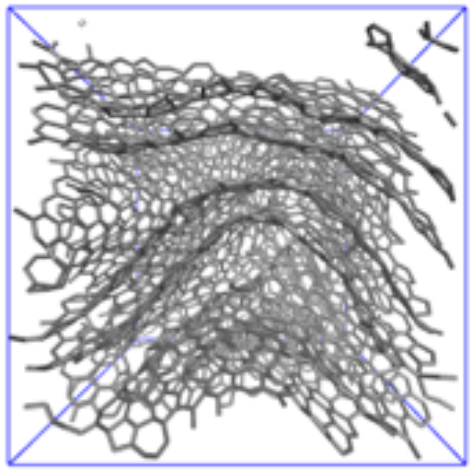
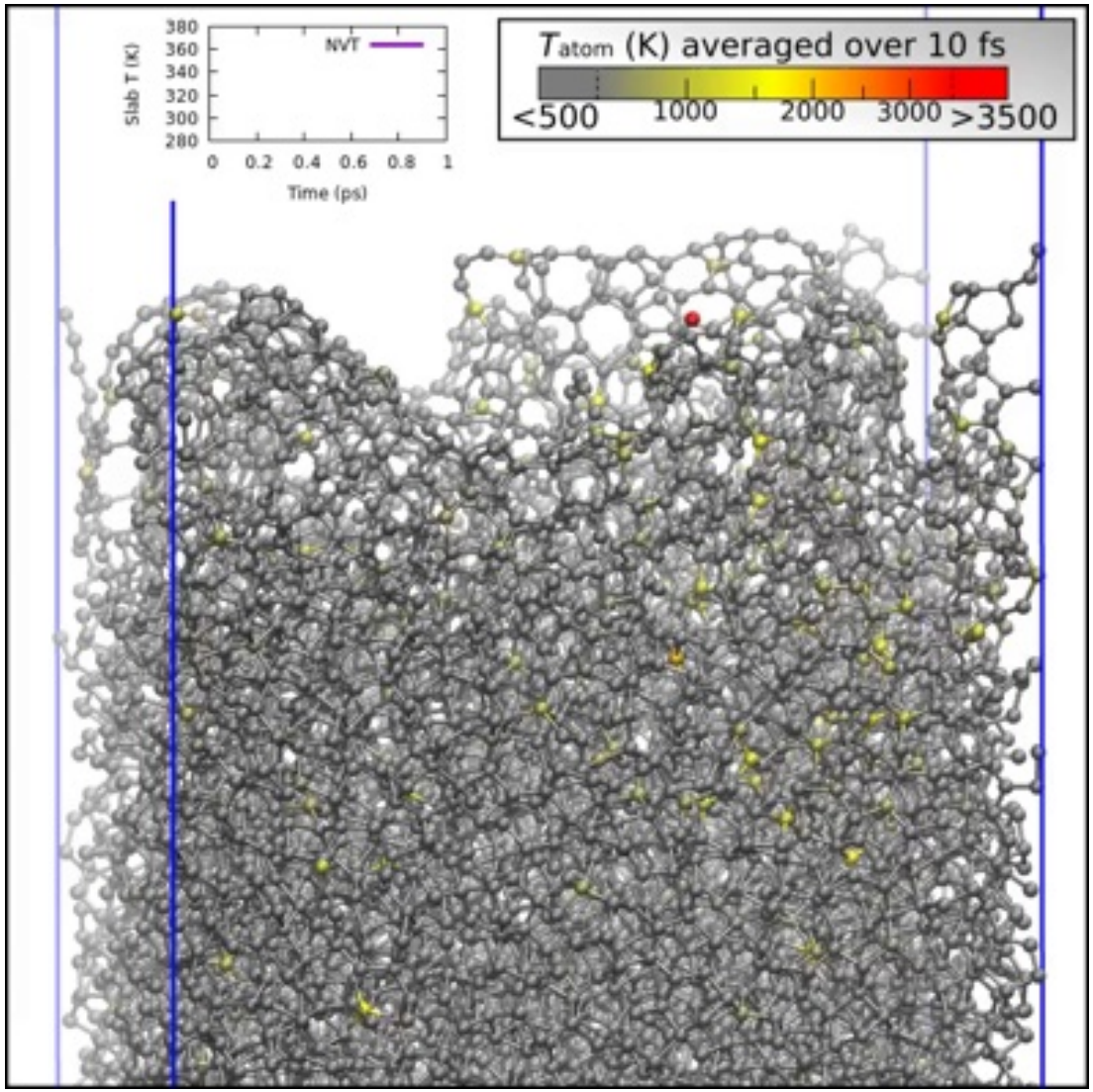
**VS**



# Amorphous carbon deposition simulations, one atom at a time




[1] M. A. Caro, G. Csányi, T. Laurila, and V. L. Deringer, Phys. Rev. B 102, 174201 (2020)

[2] M. A. Caro, Zenodo DOI:10.5281/zenodo.4000211, (2020)

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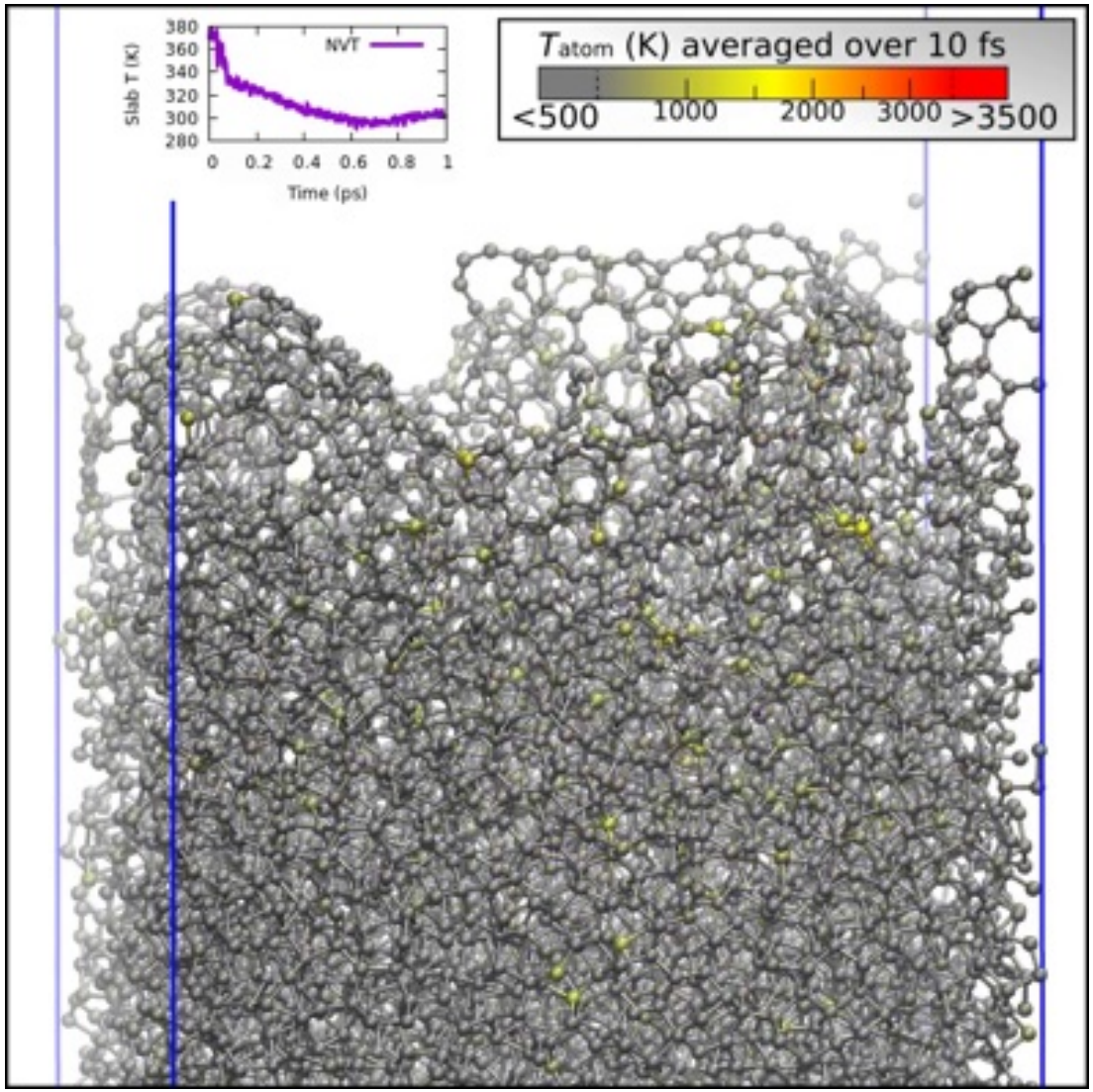
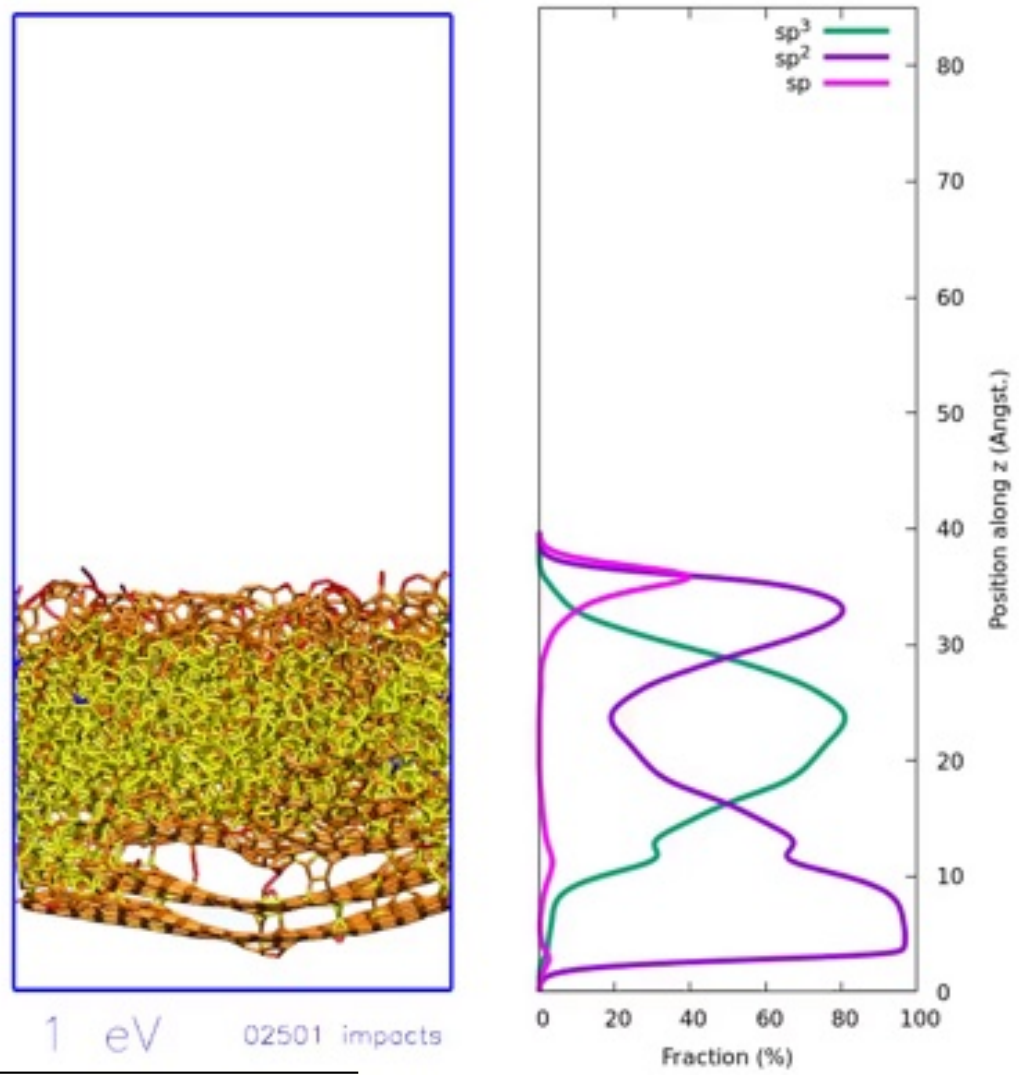



Laurila, and V. L. Deringer, Phys. Rev. B 102, 174201 (2020)

# Example 1: Amorphous carbon growth from molecular dynamics




[1] M. A. Caro, V. L. Deringer, J. Koskinen, T. Laurila, and G. Csányi, Phys. Rev. Lett. 120, 166101 (2018)

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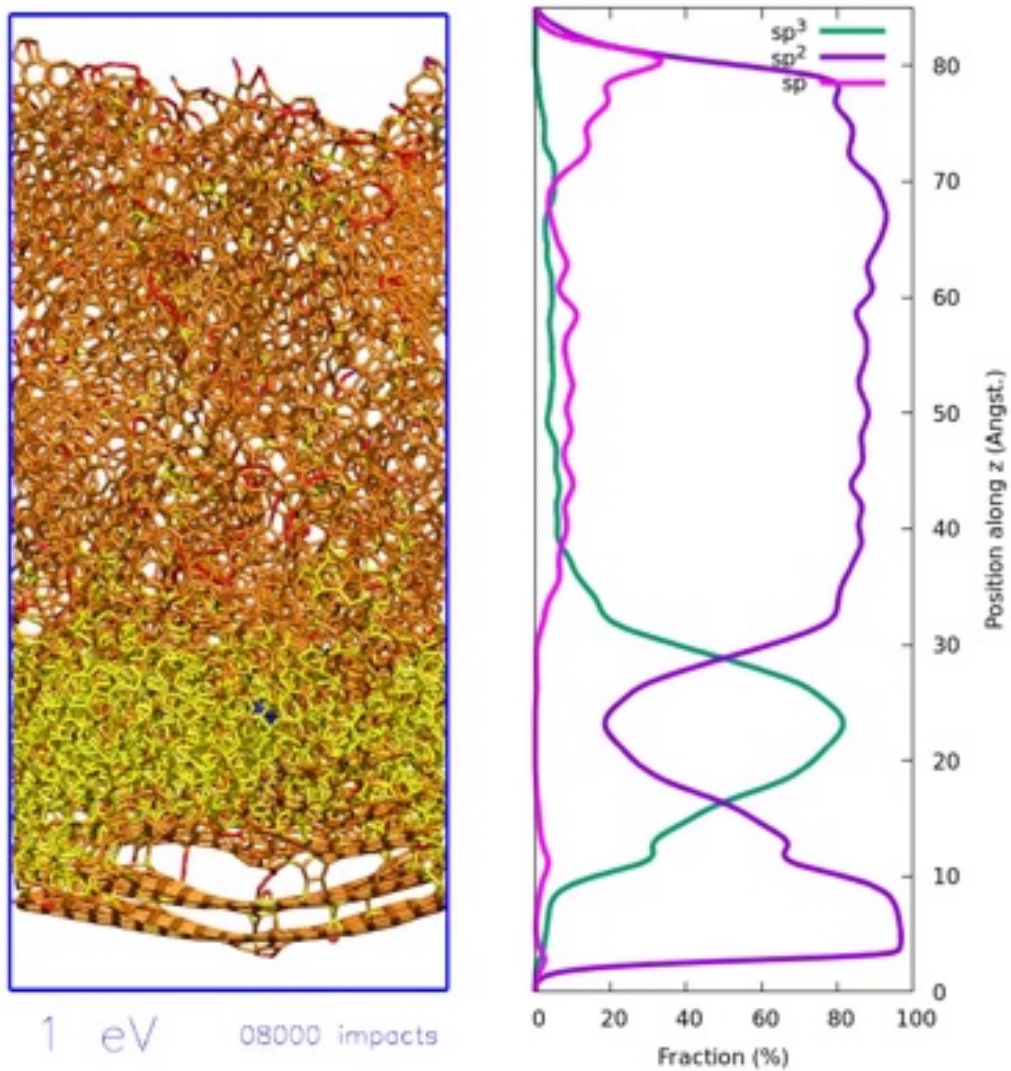


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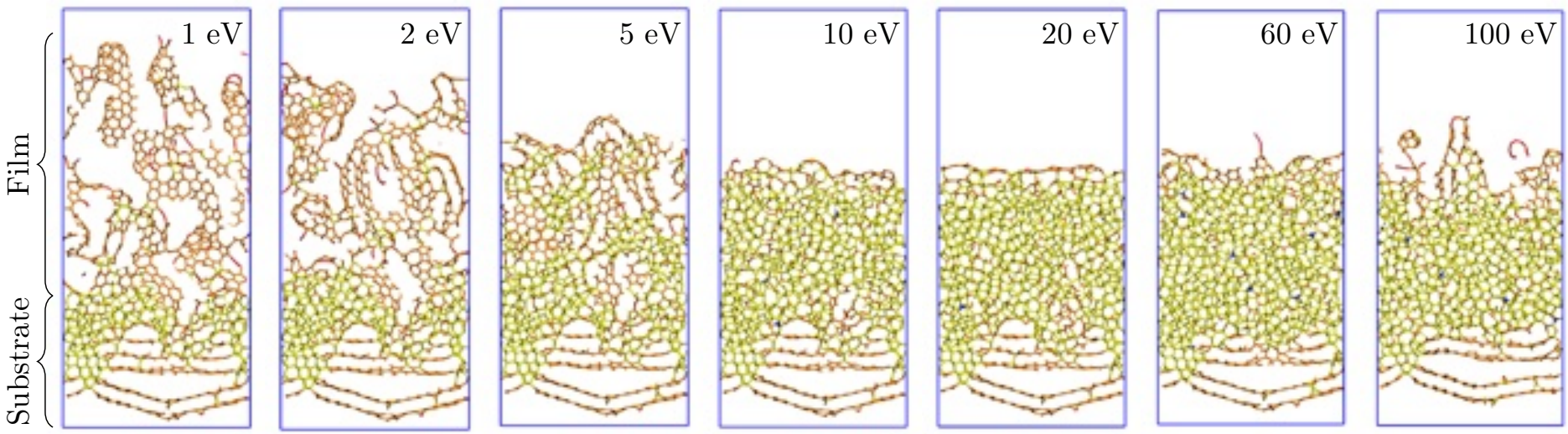
# Film characteristics

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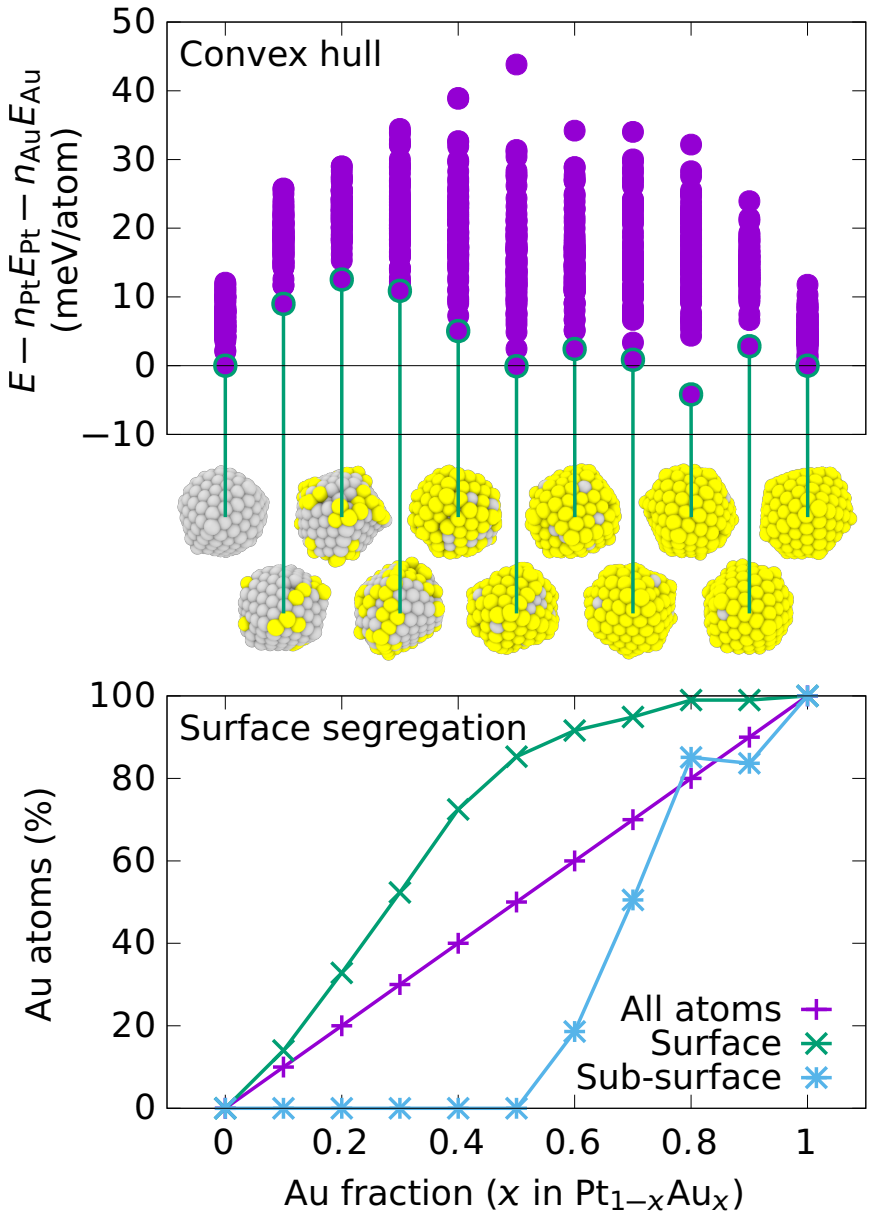
# Example 2: Enhanced H evolution reaction in PtAu:H



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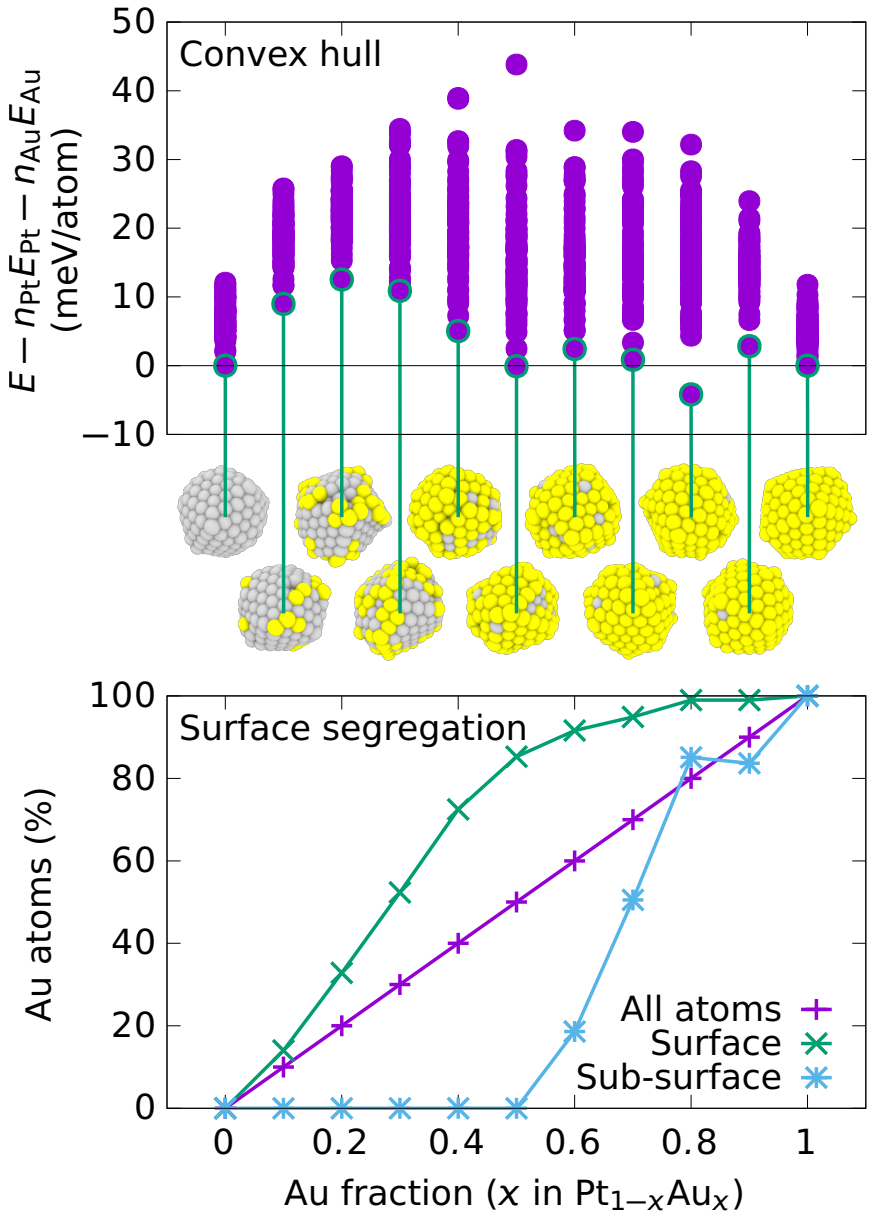


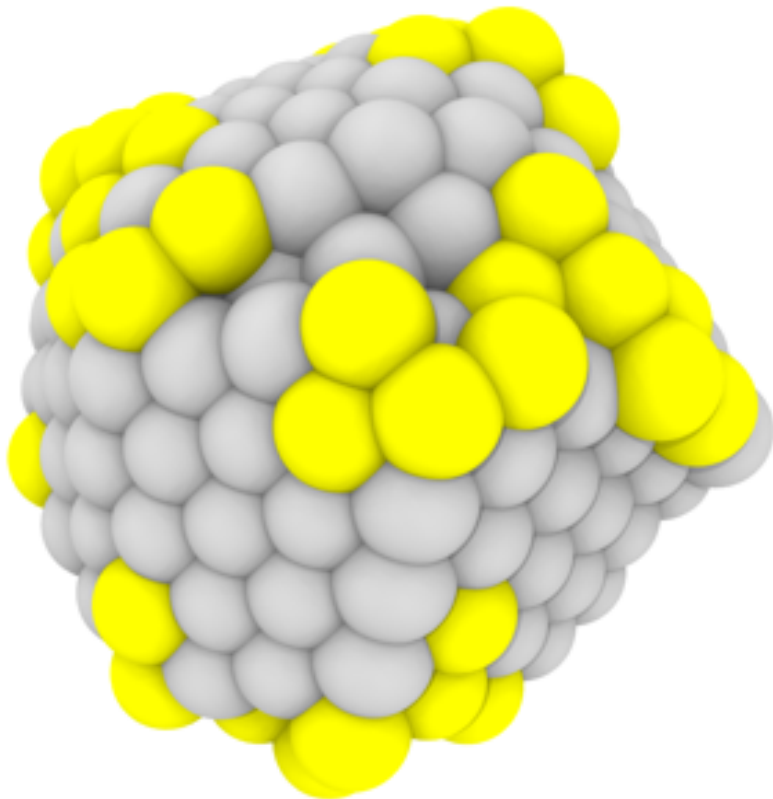

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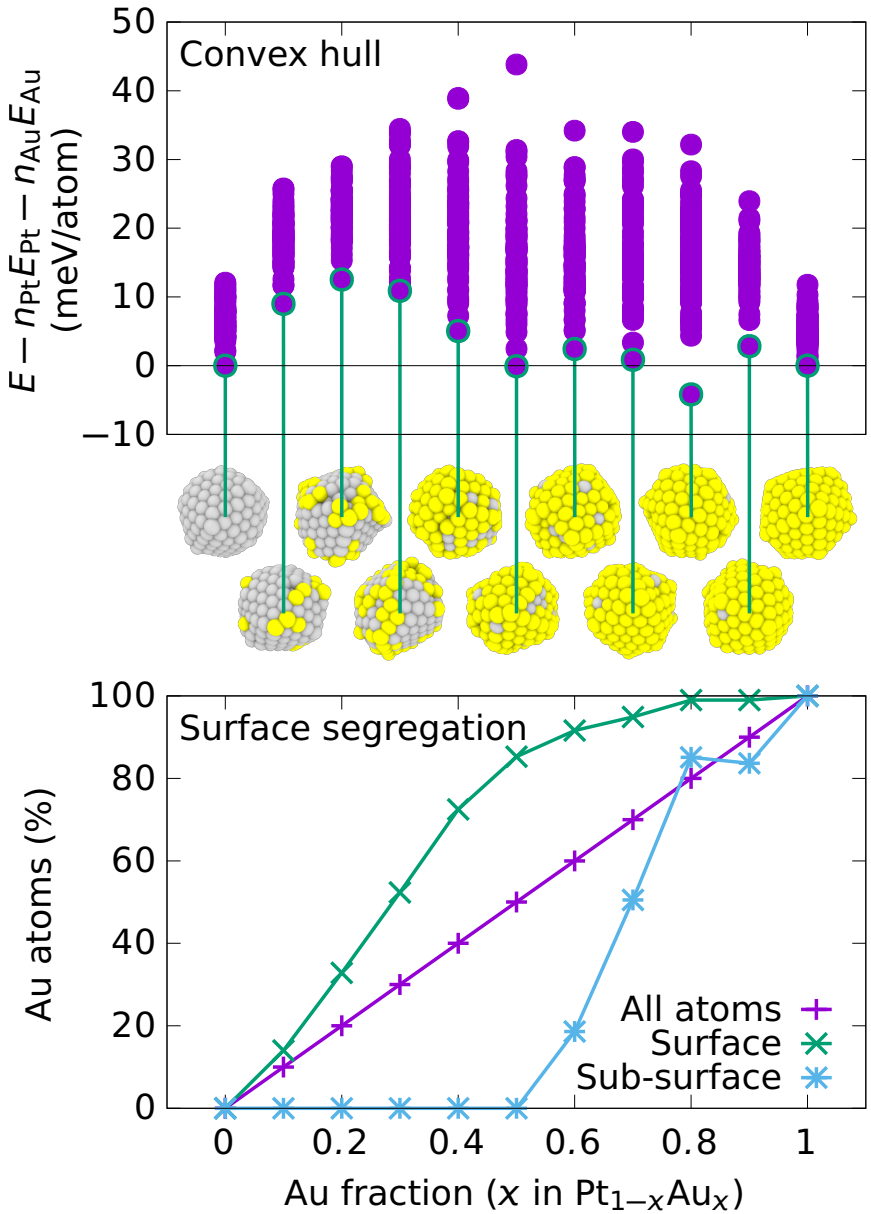


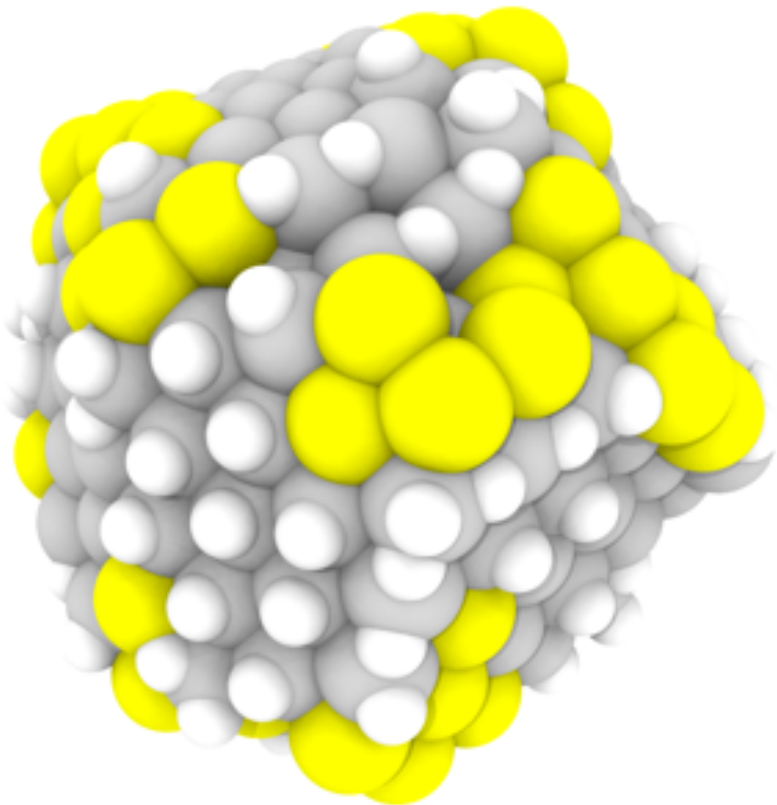

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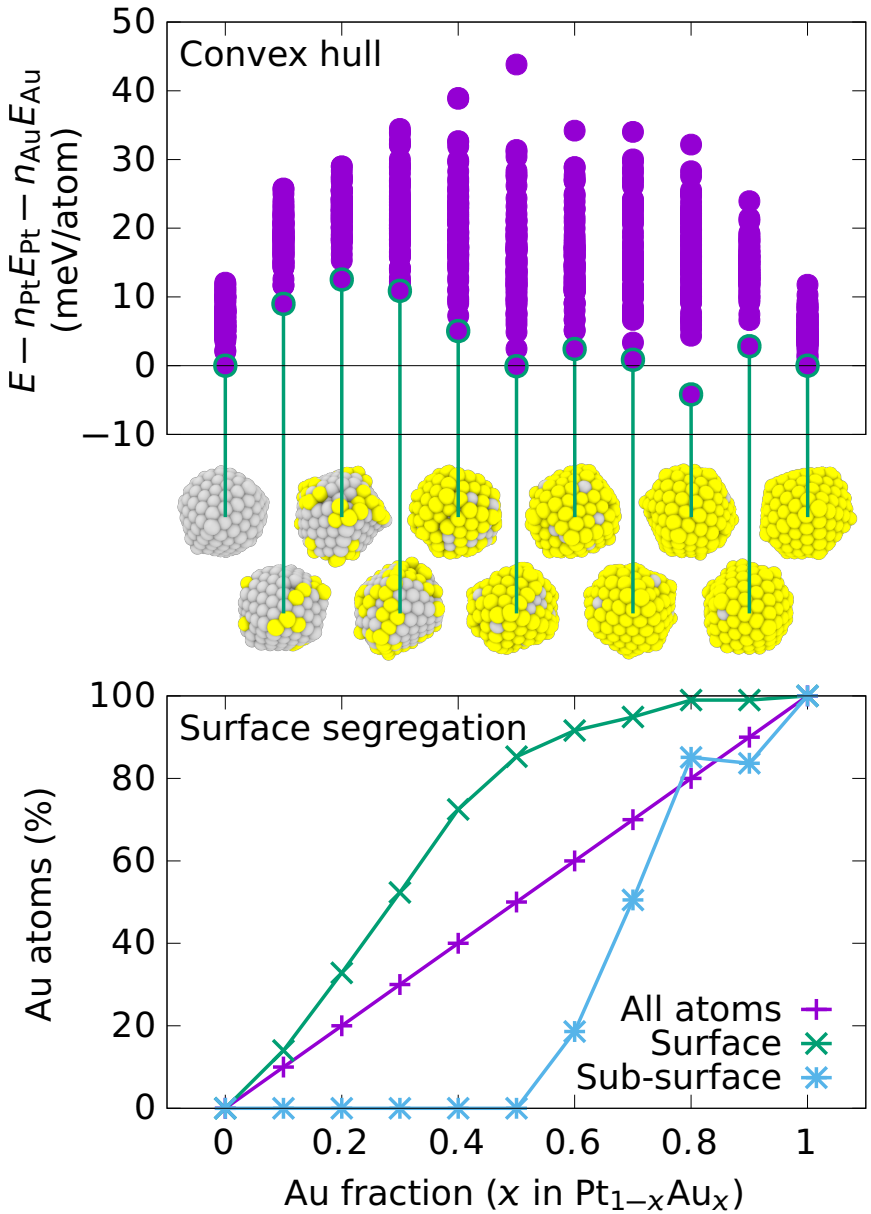
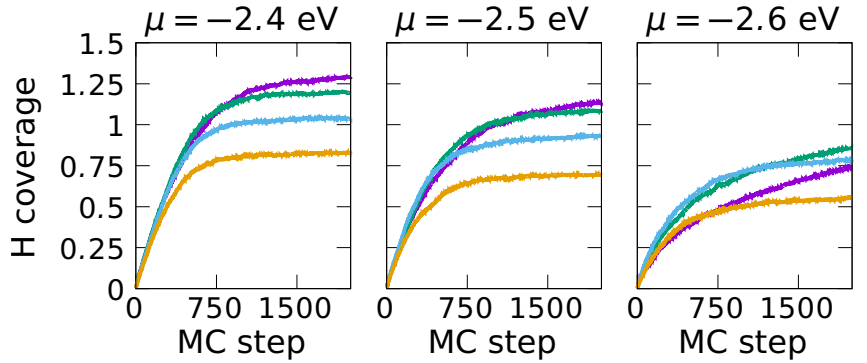
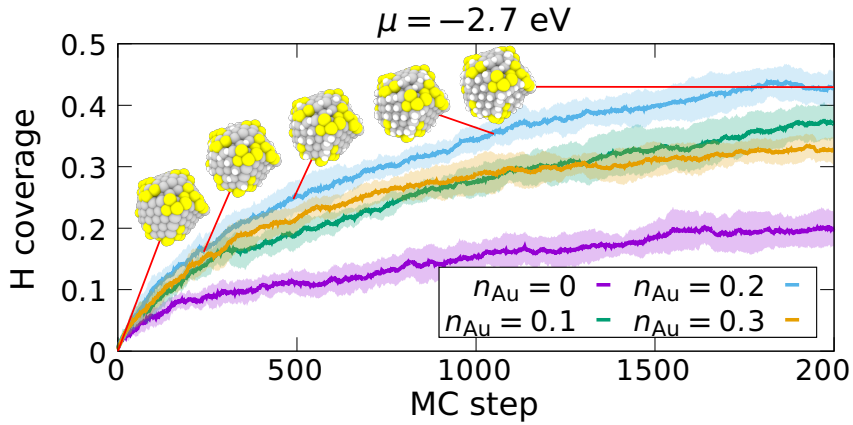
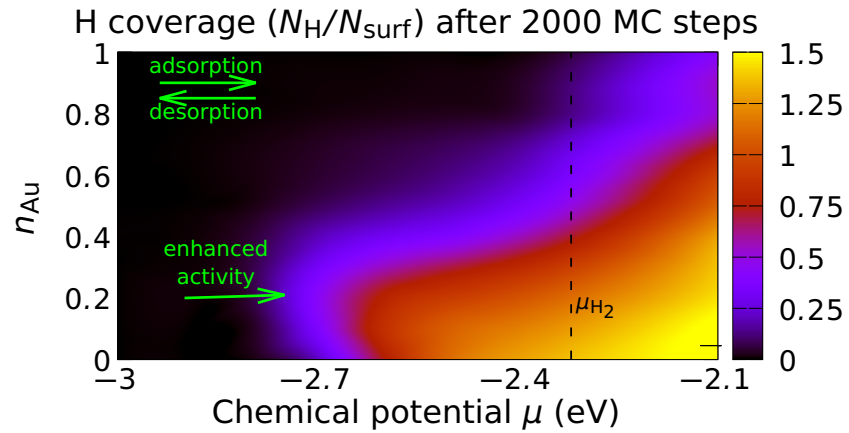
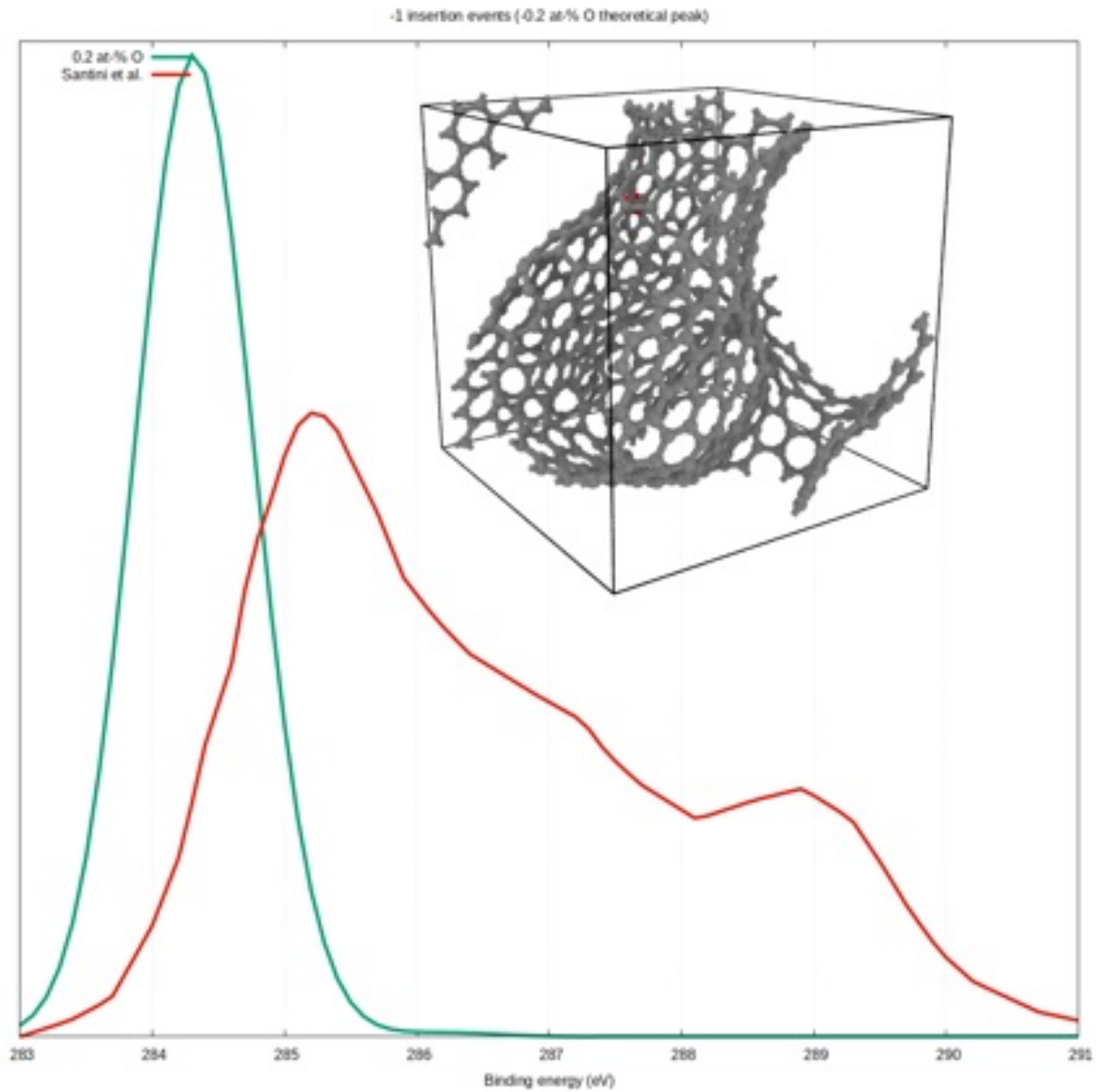


# Example 3: Experiment-driven simulation ("the future")



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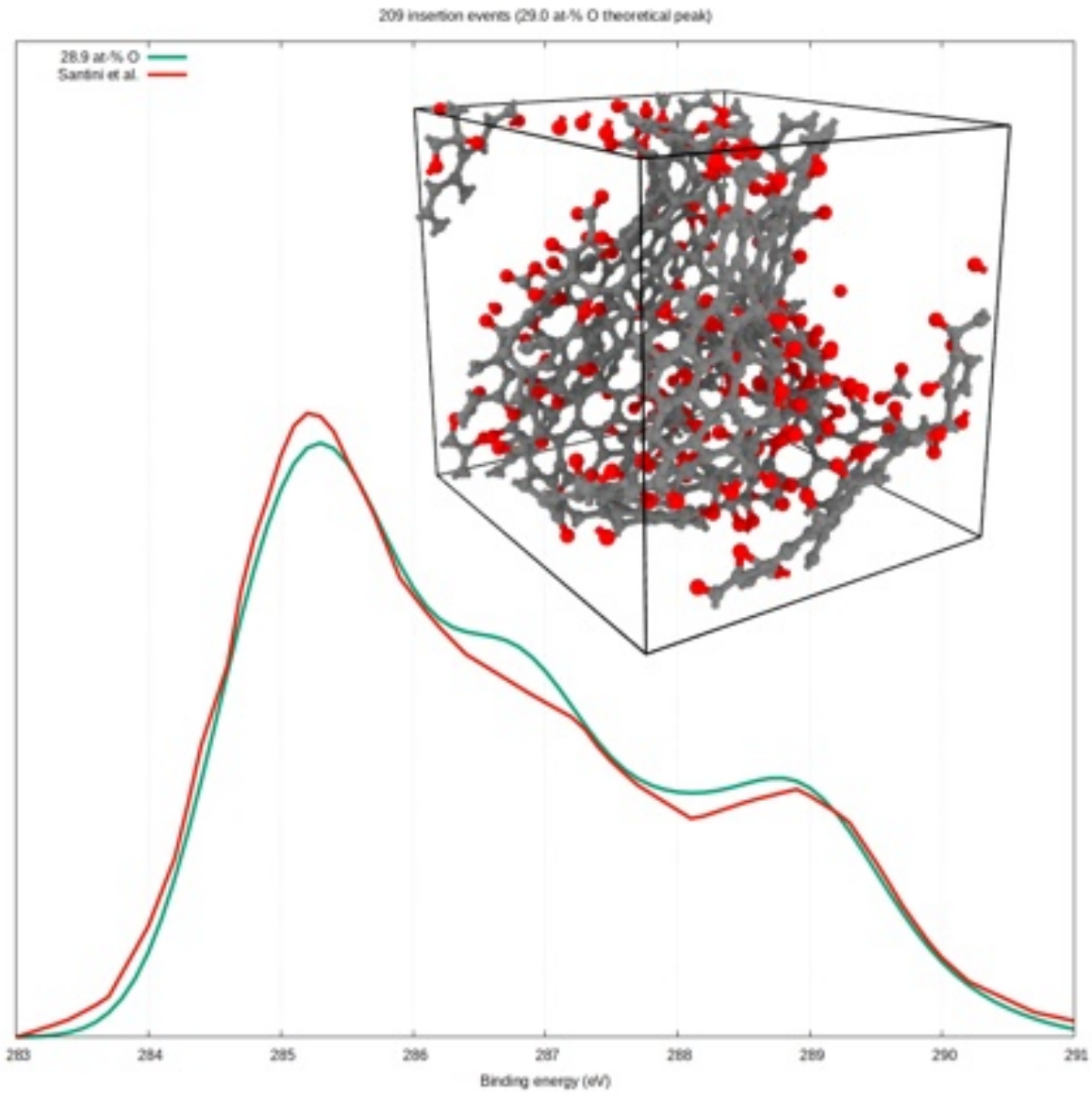


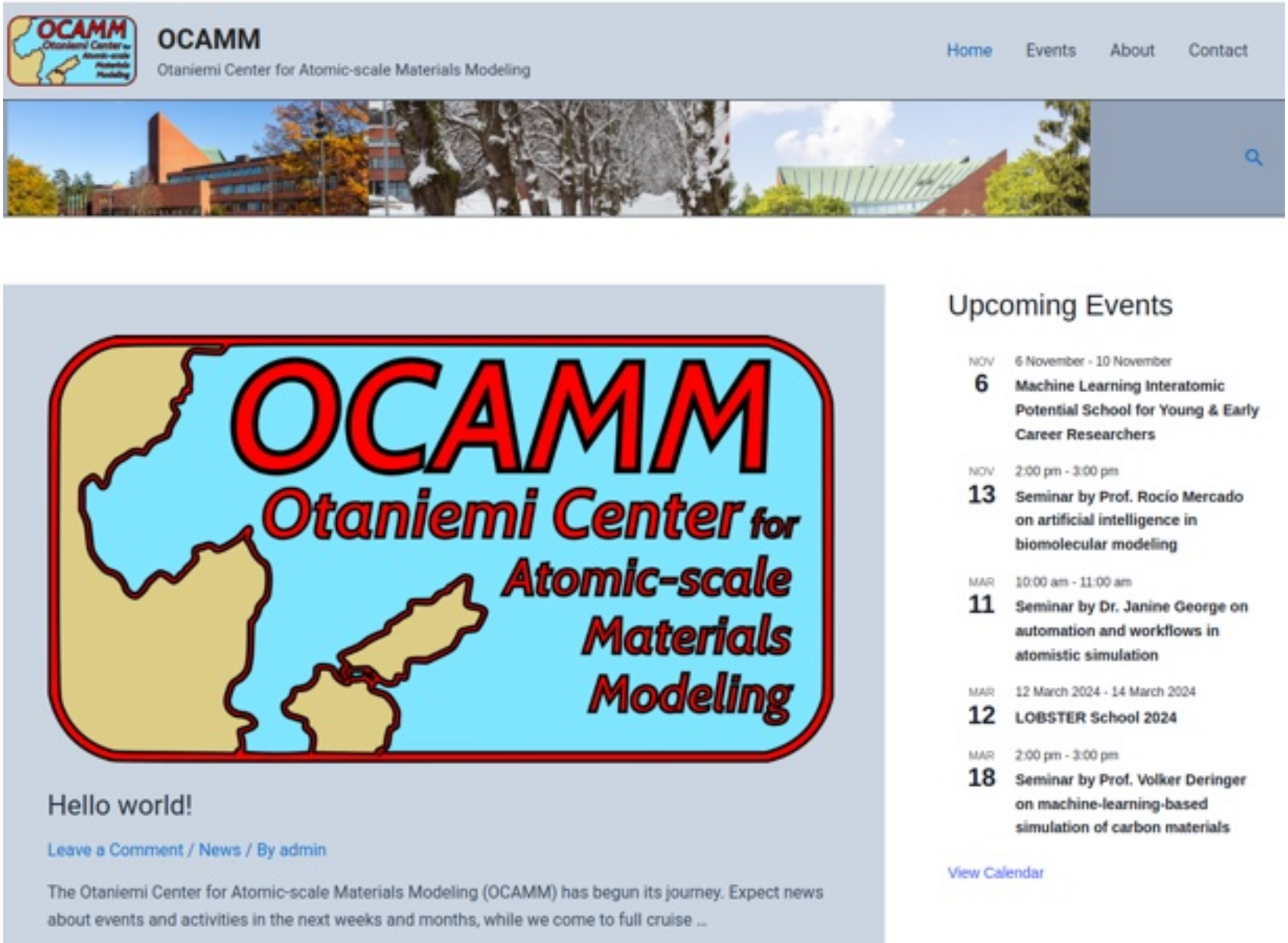
# Current status in atomistic materials modeling

- Current "explosion" in the field (methods & applications)
- Finnish HPC capabilities are very high (world-class resources)
- Finnish academia has a reasonably strong materials modeling community (although less than, e.g., Denmark & Sweden)
- My experience with industry & academic experimentalists in Finland: they are very skeptical about computational methods for materials modeling
- Adoption of atomistic modeling much lower than UK & USA
- Finnish corporations are smaller, i.e., more risk aversion ("play safe")
- Codes and methods are not (yet) "user-friendly": needs expert support
- OCAMM wants to bridge the gap between simulation experts and industry/experiment

# What's the OCAMM initiative?

- Stands for Otaniemi Center for Atomic-scale Materials Modeling
- Take advantage of the long tradition in atomistic materials modeling in Otaniemi area (Aalto and CSC)
- Bring others on board (VTT, GTK?)
- A hub to coordinate the activities in atomistic materials modeling: research, education and innovation, including software development and optimization (e.g., enable GPU readiness)
- Increase the presence of simulation in predominantly experimental (academic) projects
- Gateway for industry. We will help you:
  - Assess the relevance of materials simulation for your innovation problem
  - Find relevant experts among OCAMM partners
  - Facilitate cooperation via simplified and centralized procedures (e.g., pro forma contracts)
- Assist in the incorporation of simulation WPs to funding proposals (AKA, EU, BF, etc.)
- We're getting started: currently raising awareness, securing funding, and organizing events

# ocamm.fi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The Otaniemi Center for Atomic-scale Materials Modeling (OCAMM) has begun its journey. Expect news about events and activities in the next weeks and months, while we come to full cruise ...
Upcoming Events
NOV 6 6 November - 10 November
Machine Learning Interatomic Potential School for Young & Early Career Researchers
NOV 13 2:00 pm - 3:00 pm
Seminar by Prof. Rocío Mercado on artificial intelligence in biomolecular modeling
MAR 11 10:00 am - 11:00 am
Seminar by Dr. Janine George on automation and workflows in atomistic simulation
MAR 12 12 March 2024 - 14 March 2024
LOBSTER School 2024
MAR 18 2:00 pm - 3:00 pm
Seminar by Prof. Volker Deringer on machine-learning-based simulation of carbon materials
View Calendar