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Long-Time Scale Molecular Dynamics of Large-Scale Simulations Enhanced by Machine Learning of Hydroxylated Tin Oxide

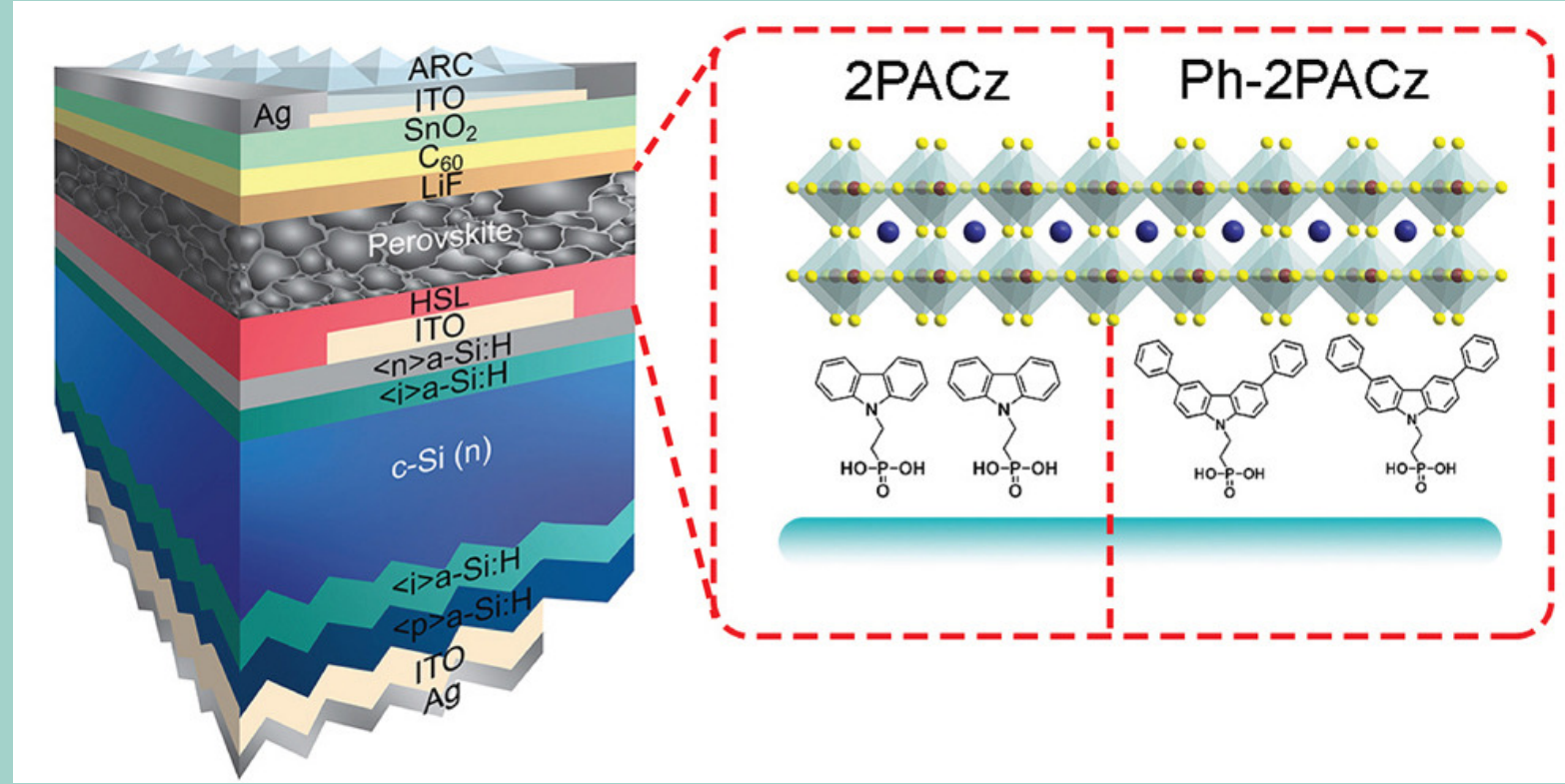
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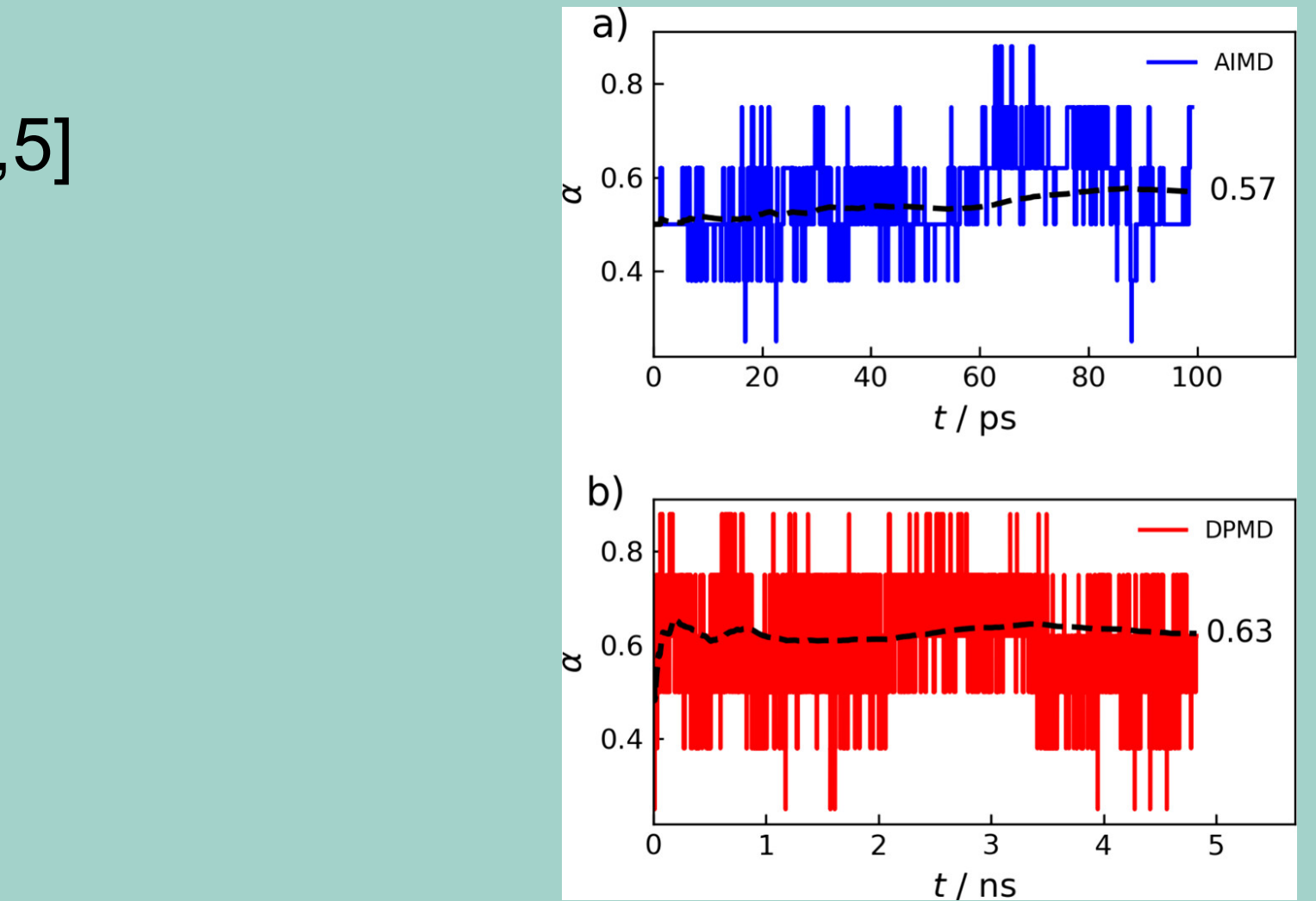
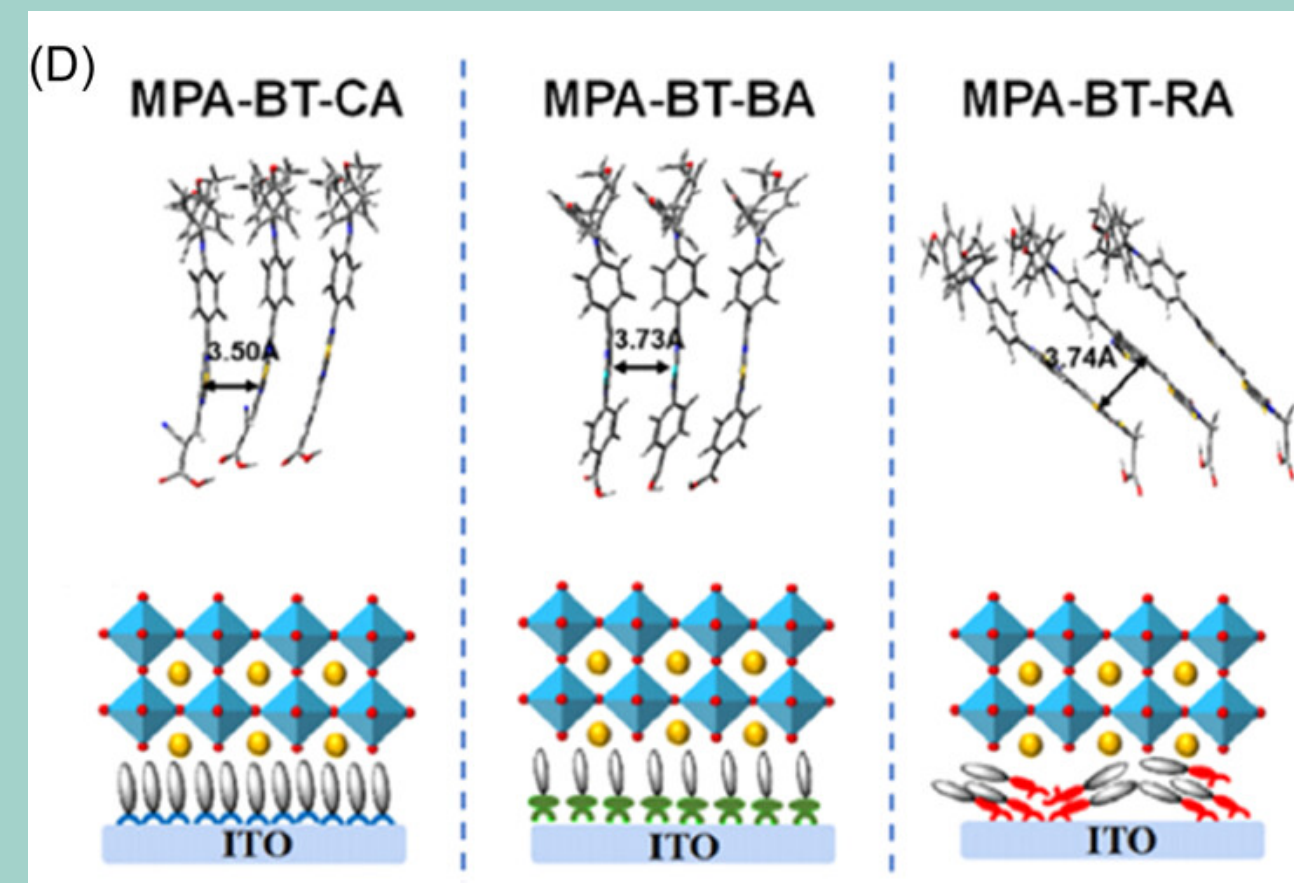
LCBC
Laboratoire de Chimie et Biochimie
Computationnelles

1 Doped Tin Oxide (SnO_2) is used as HTL in perovskite solar cell [1,2]



2 To prevent degradation and to improve the HTL-AL interface it can be passivated

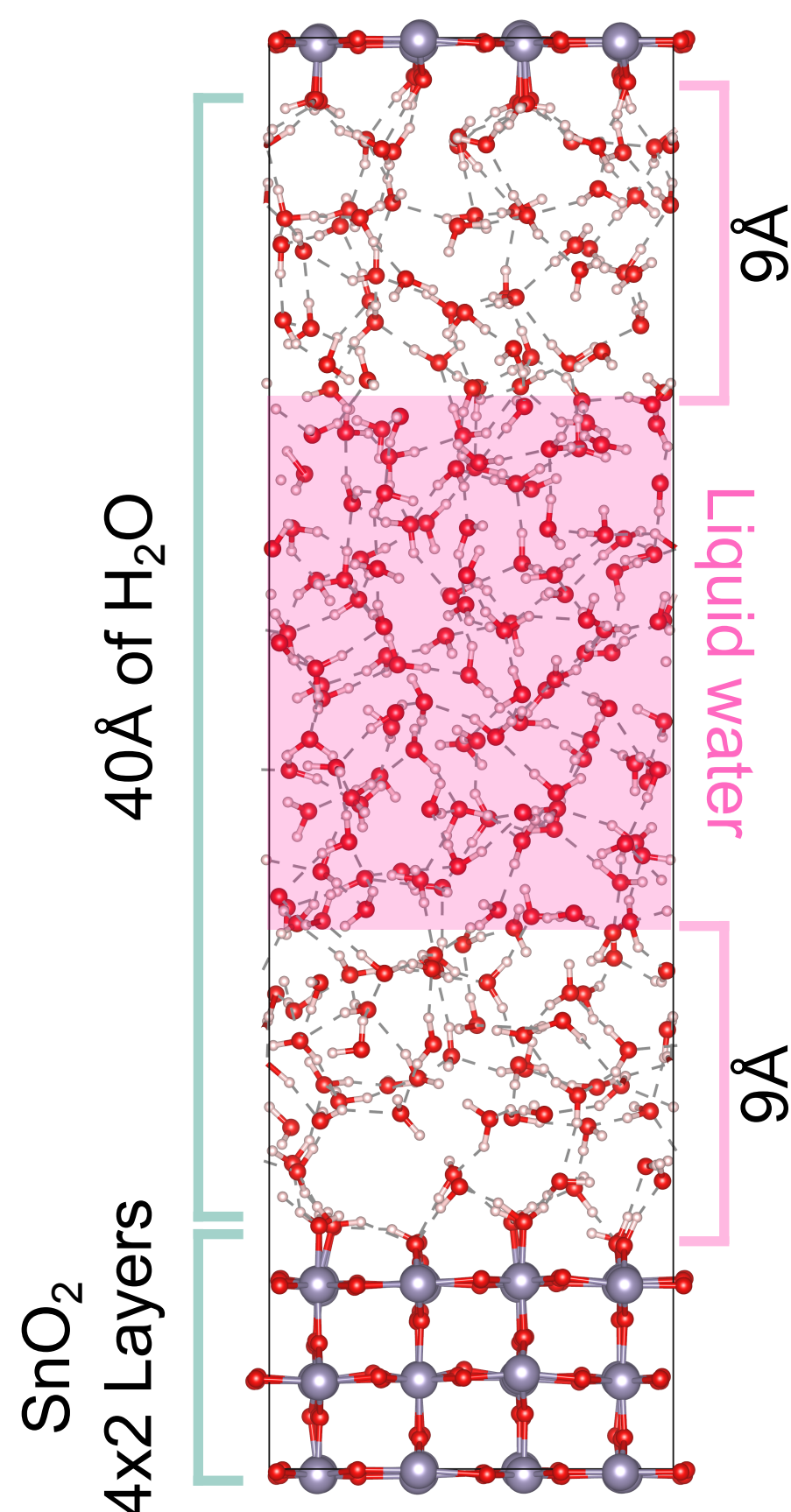
3 Additives serve as junction between HTL and perovskite [3,4,5]



4 Proton transfer is a long time scale process so we need long dynamics on large system [6,7]

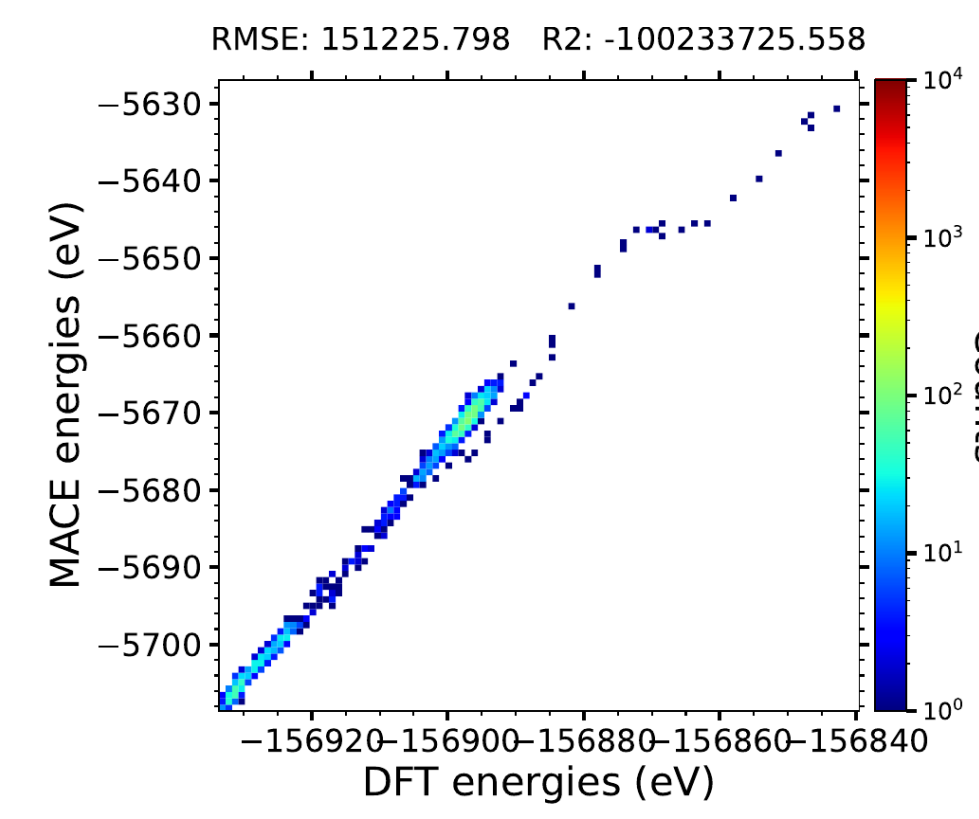
PREPARATION

- 1 **CP2K**
- DFT PARAMETERS
- r2SCAN + Grimme D3
GTH pseudopotential
O: TZVP, H/Sn: DZVP
- 1x10ps AIMD at 300K
5x2ps AIMD at 500K



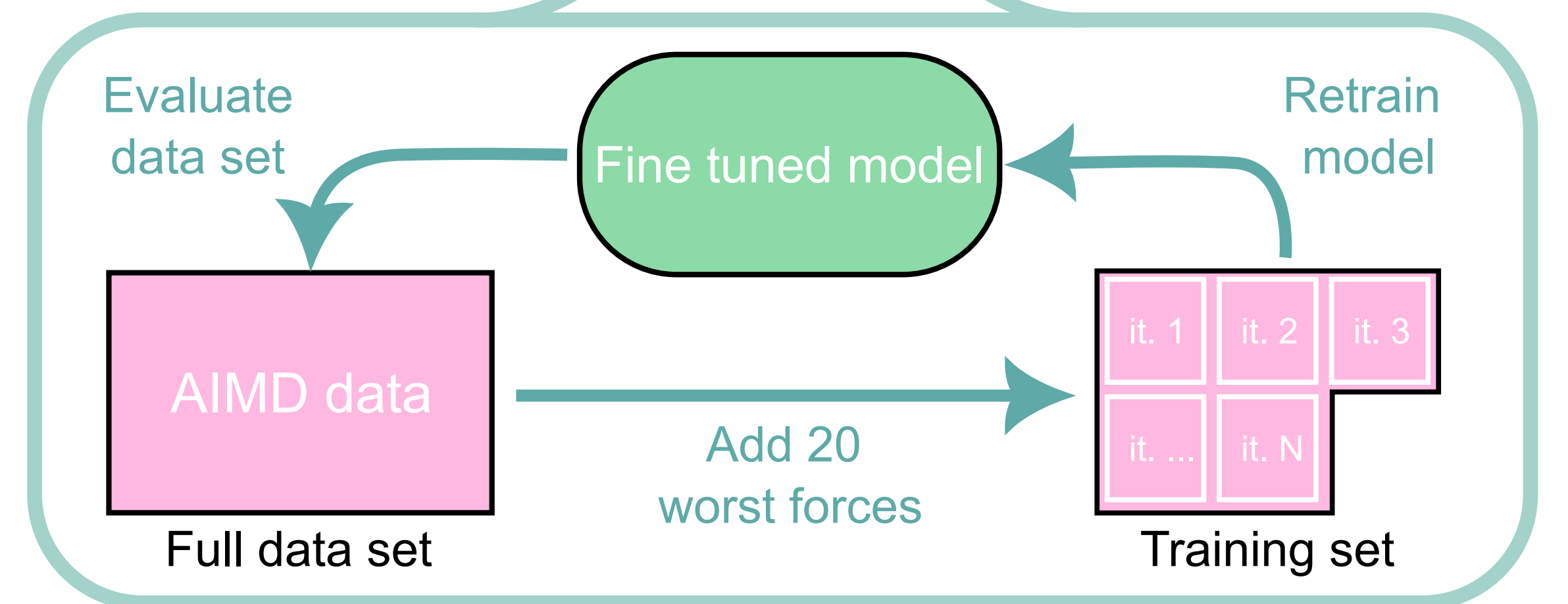
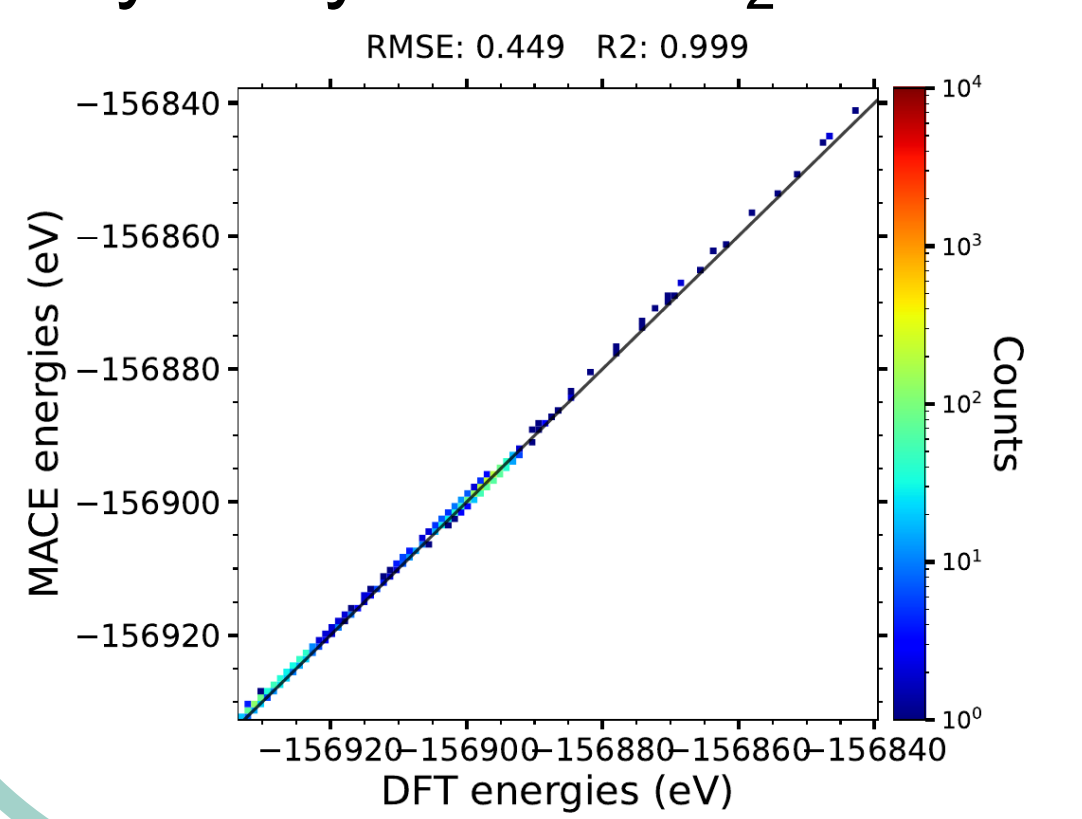
- 2 **MACE**
- MLIP PARAMETERS
- Irreps 128x0e+128x1o
 - 2 layers
 - Correlation order: 3
 - Radial cutoff: 6.0 Å
 - Total nb of parameters: 752174
 - Nb of gradient updates: 3600
- Training set: 8x20 conf.
RMSE(E) = 0.5 meV/atom
RMSE(F) = 38.7 meV/Å

matpes-r2SCAN foundation

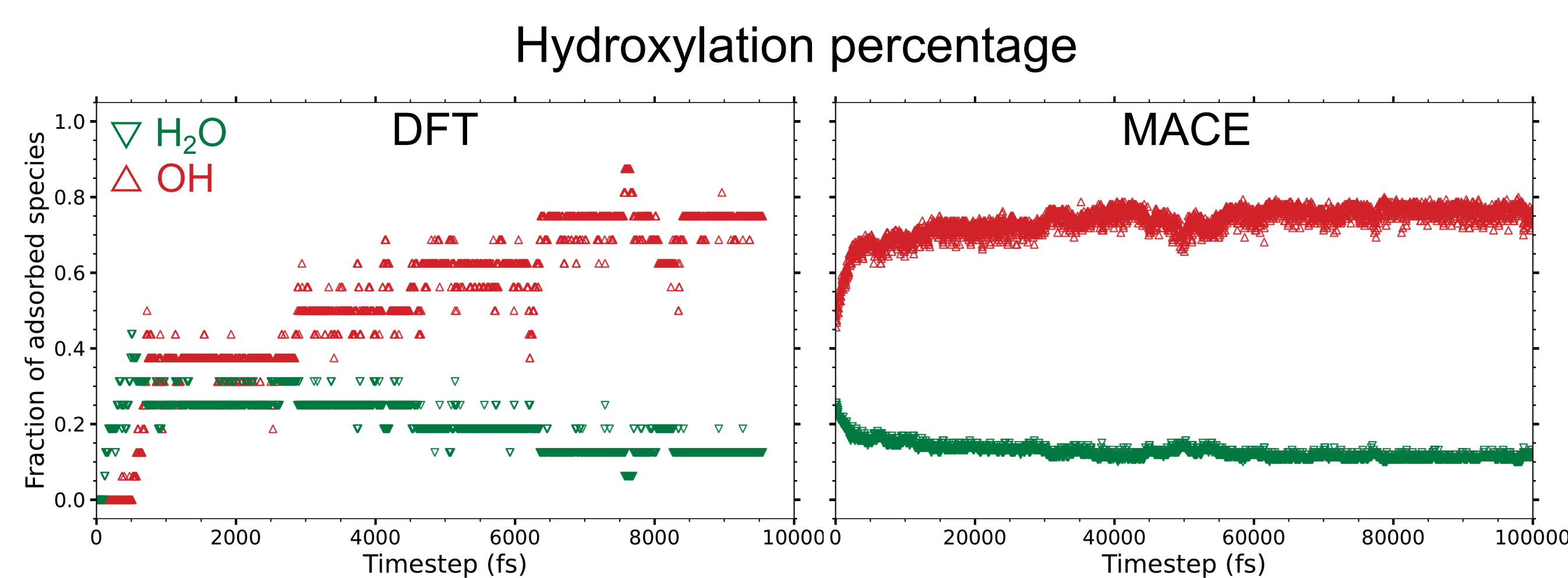
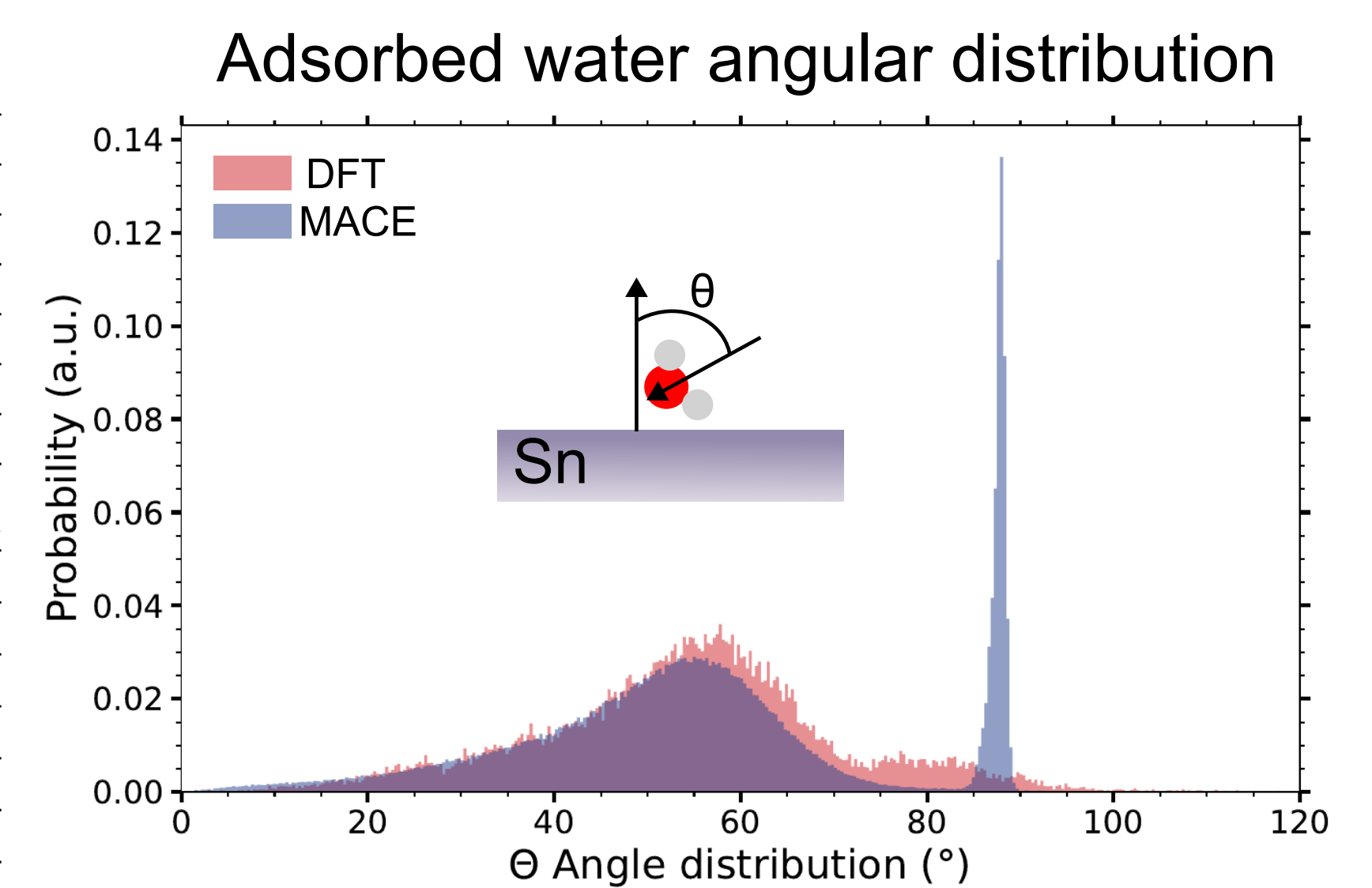
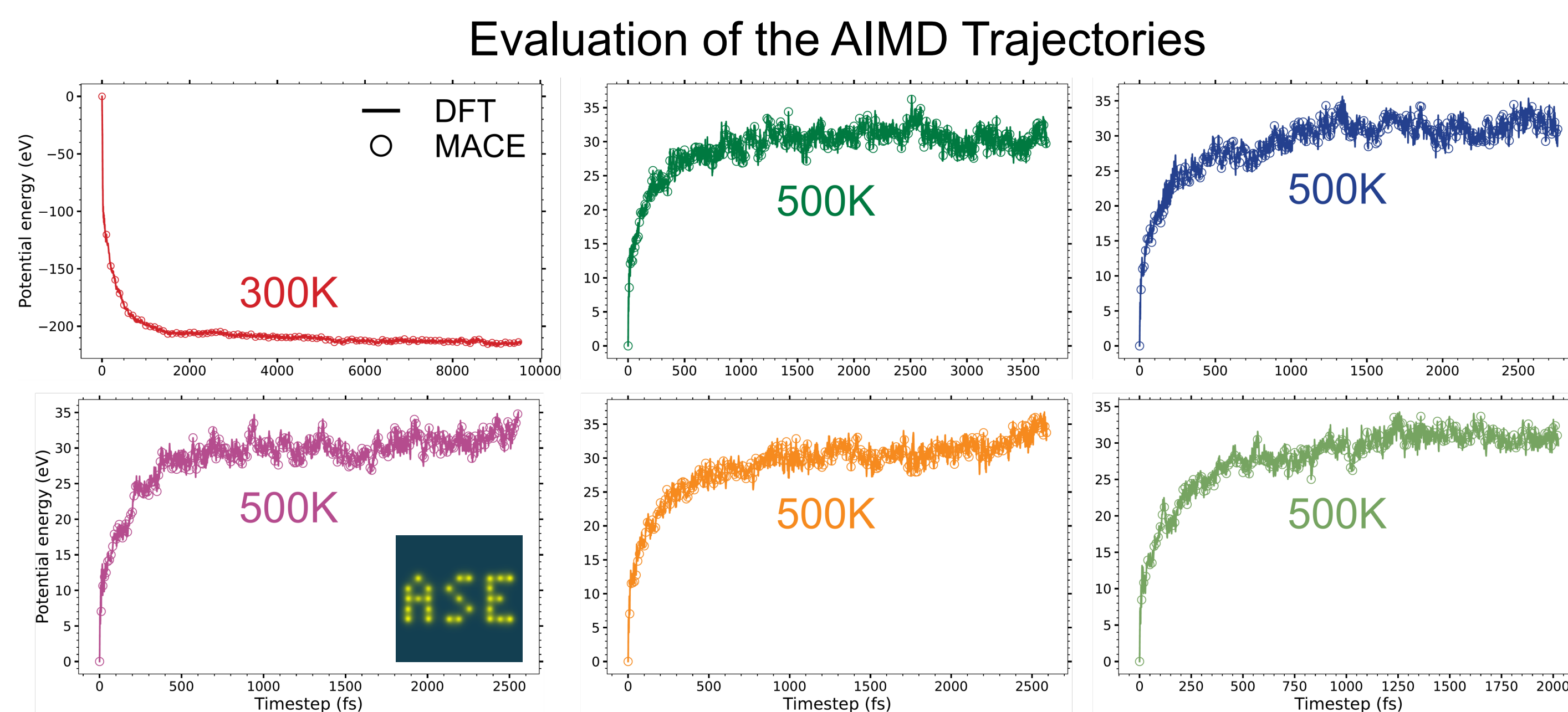
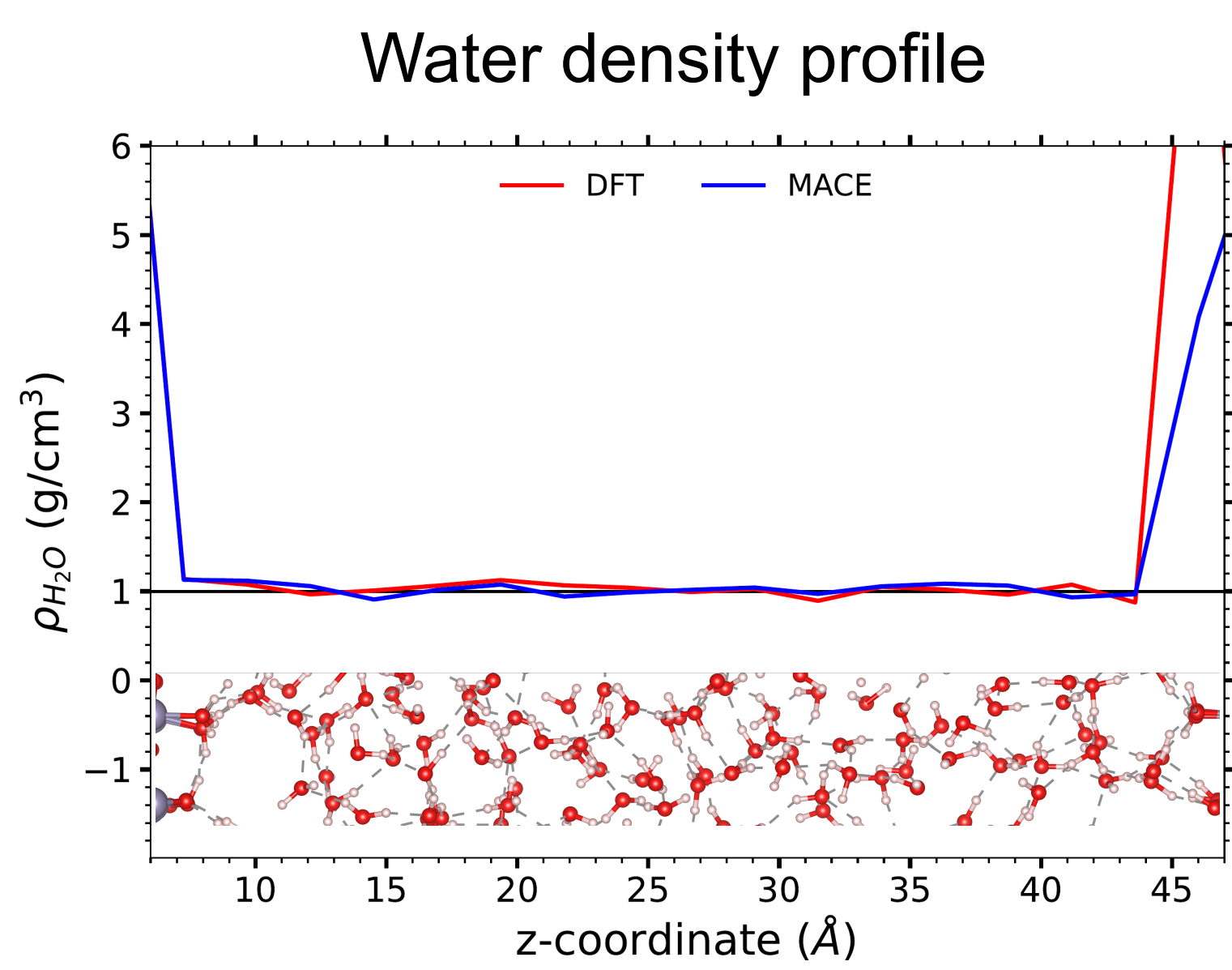


Naive finetuning
Active learning

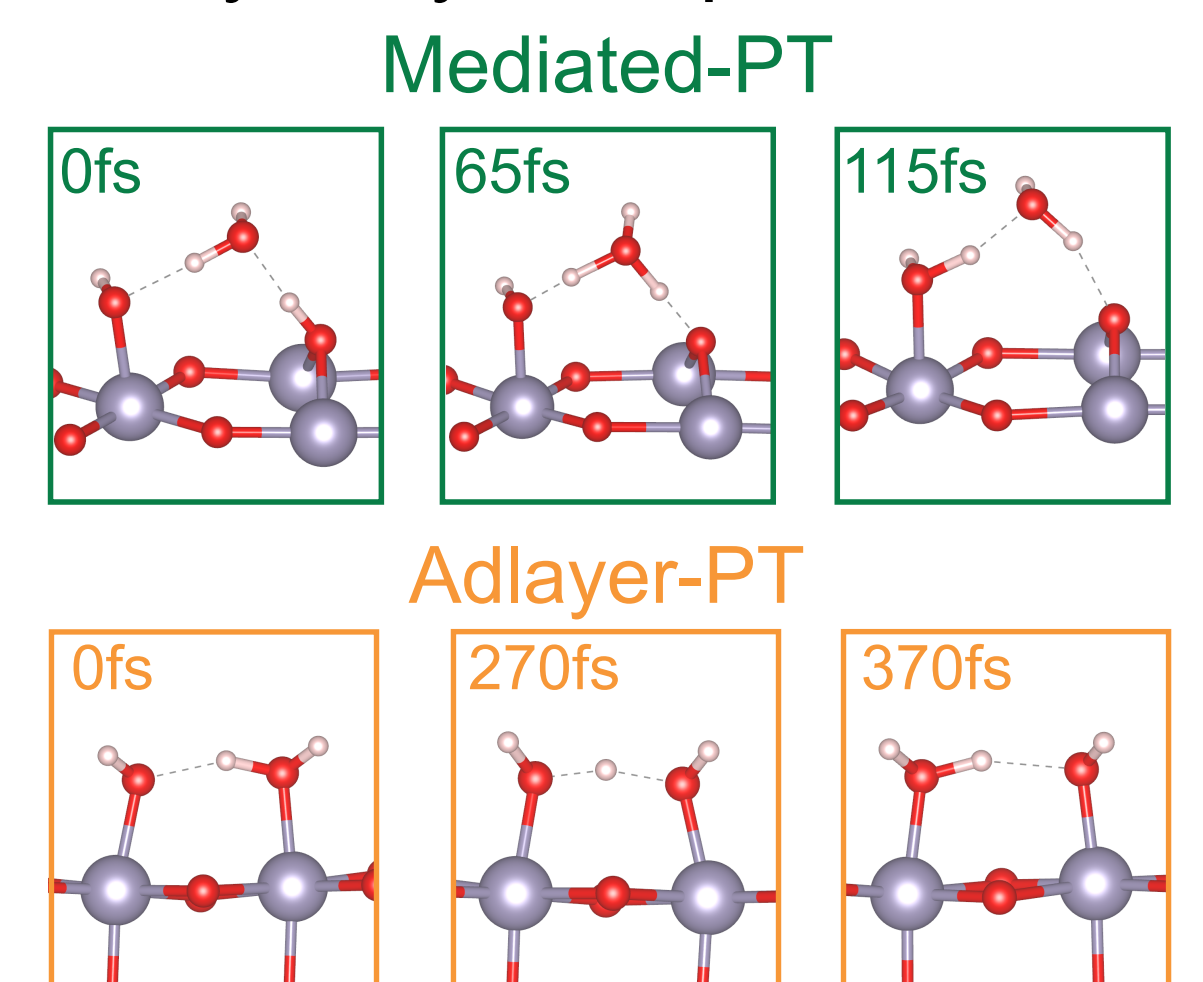
Hydroxylated SnO_2 model



RESULTS

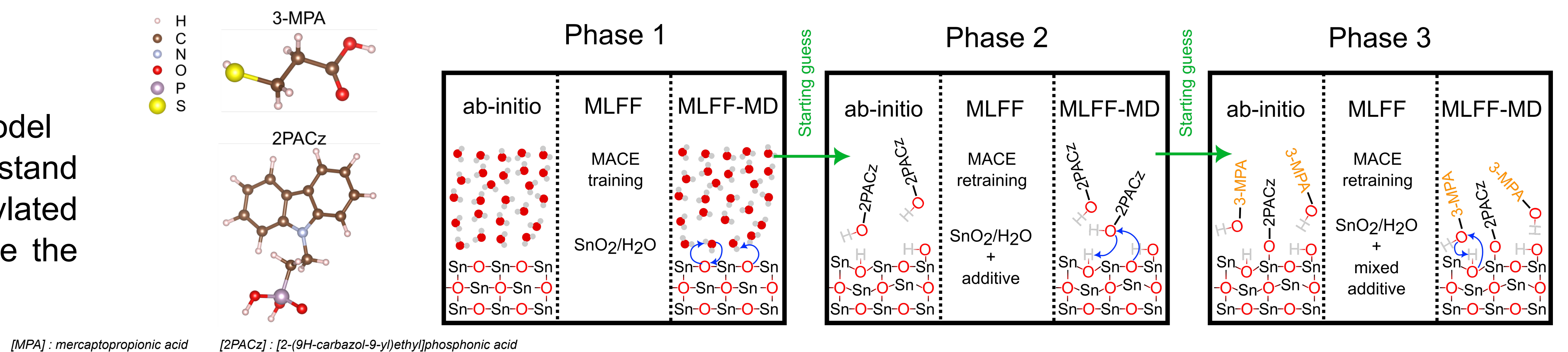


Hydroxylation processes



PERSPECTIVES

- Add additives to the MLIP model
- Compute ML-MD and understand the reactions between hydroxylated SnO_2 and additives to enhance the efficiency of solar cell devices



[MPA]: mercaptopropionic acid [2PACz]: [2-(9H-carbazol-9-yl)ethyl]phosphonic acid

[1] G. Wang et al. *Joule* 7, 2583 (2023) [2] P. Han et al. *Advanced Materials* 36, 2405630 (2024)
 [3] Q. Liao et al. *Journal of Energy Chemistry* 68, 87 (2022) [4] Z. Yi et al. *Interdisciplinary Materials* 3, 203 (2024) [5] S. M. Park et al. *Nature* 624, 289 (2023)
 [6] X.-T. Fan et al. *Journal of Energy Chemistry* 82, 239 (2023) [7] M. Jia et al. *Precision Chemistry* 2, 644 (2024)
 CP2K: T. D. Kühne et al. *J. Chem. Phys.* 152, 19 (2020)
 MACE: I. Batatia et al. arXiv:2206.07697 (2022) Foundation model: I. Batatia et al.: arXiv:2401.00096 (2023)
 matpes: A. D. Kaplan et al. arXiv:2503.04070 (2025)
 ASE: A. H. Larsen et al. *J. Phys. Condens. Matter* 29, 273002 (2017)



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Any Questions?
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