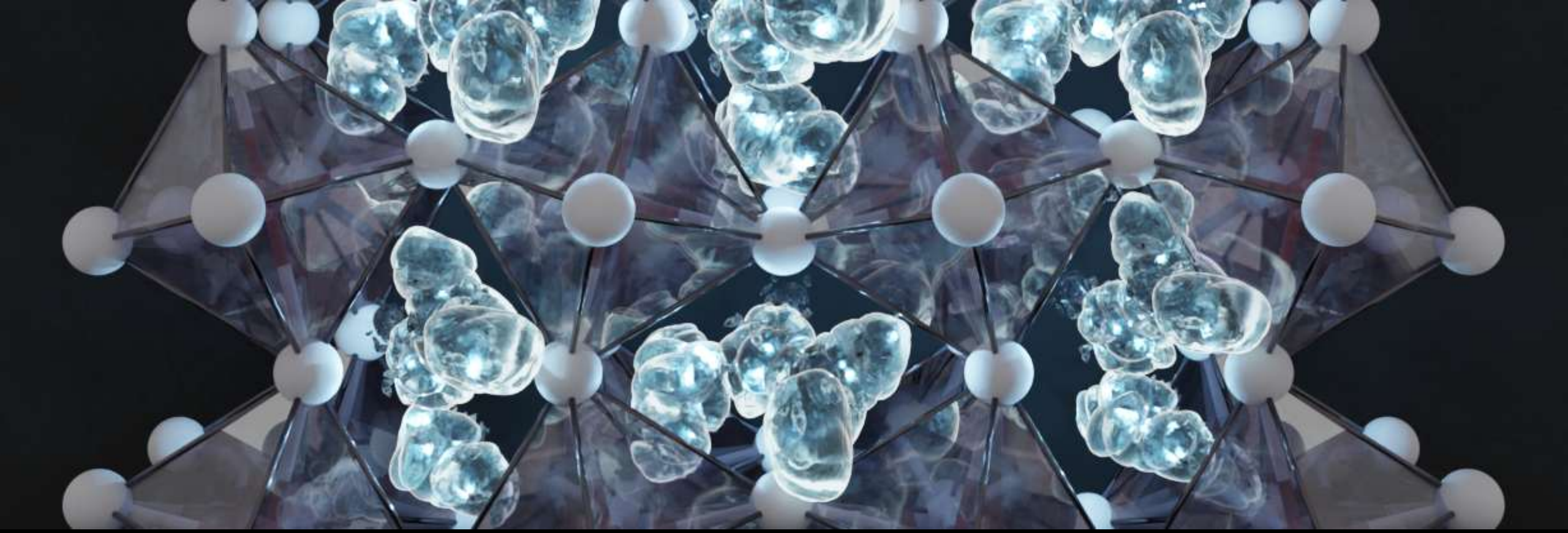

Toward Better Materials for Solar Energy through Advanced Modeling

Julia Wiktor

Department of Physics, Chalmers

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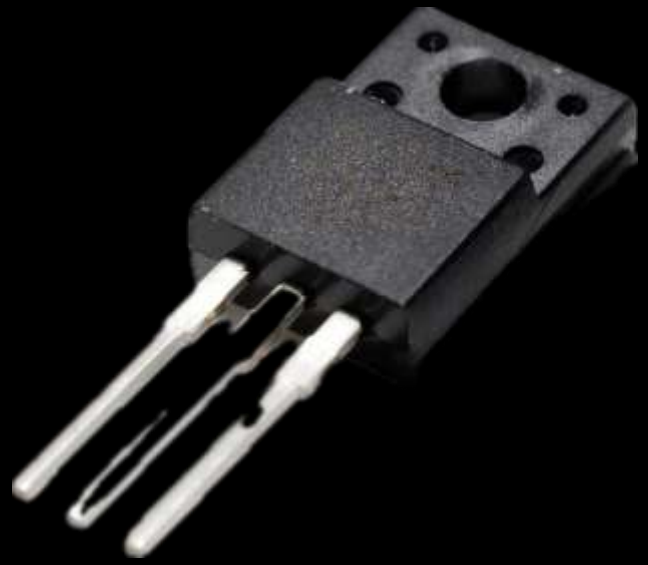
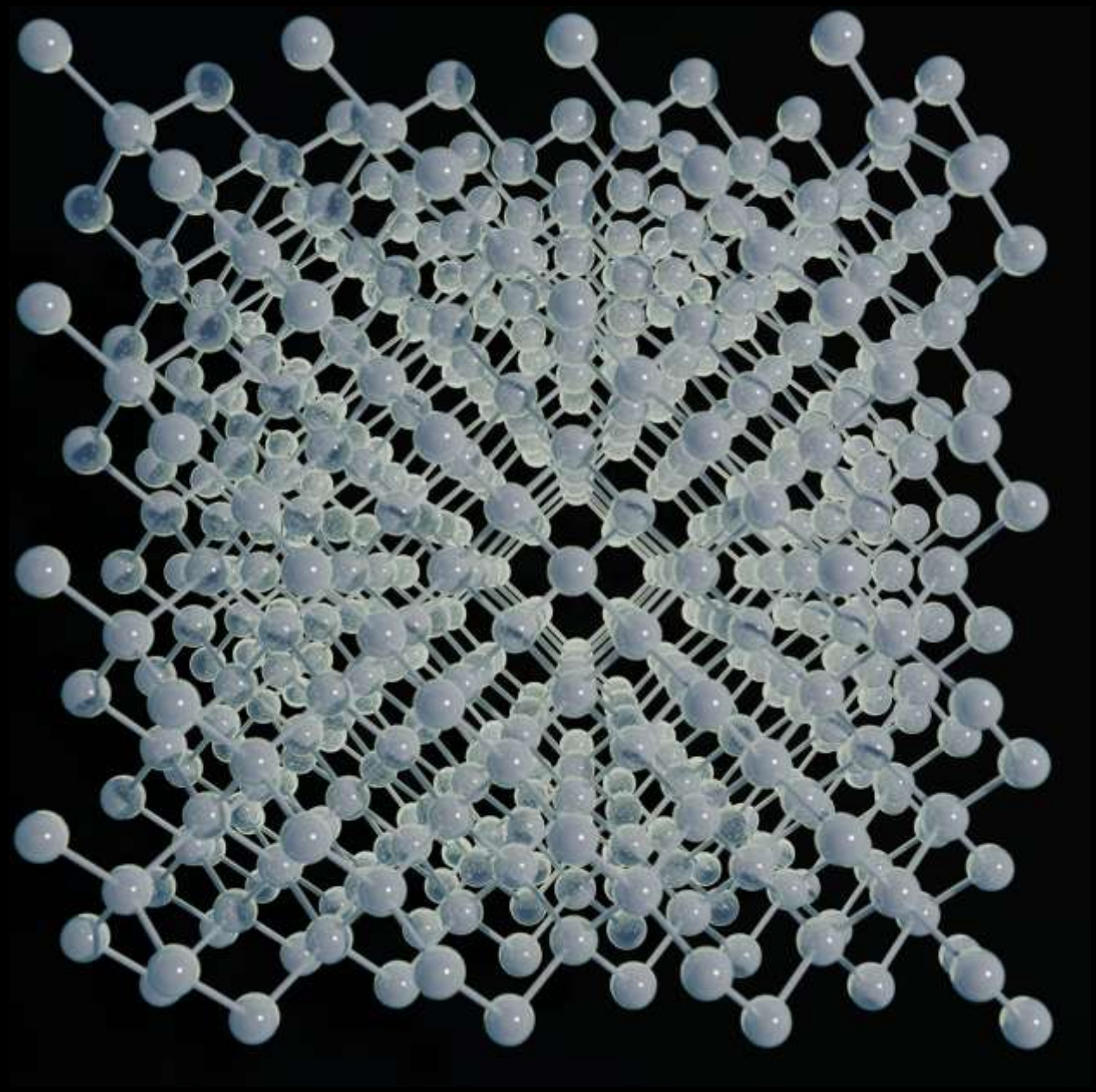


Silicon



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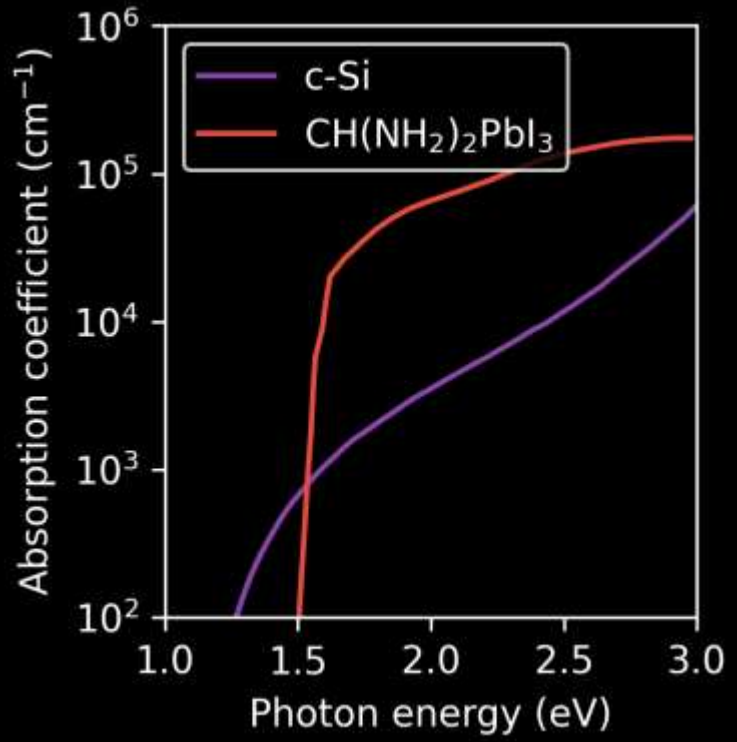
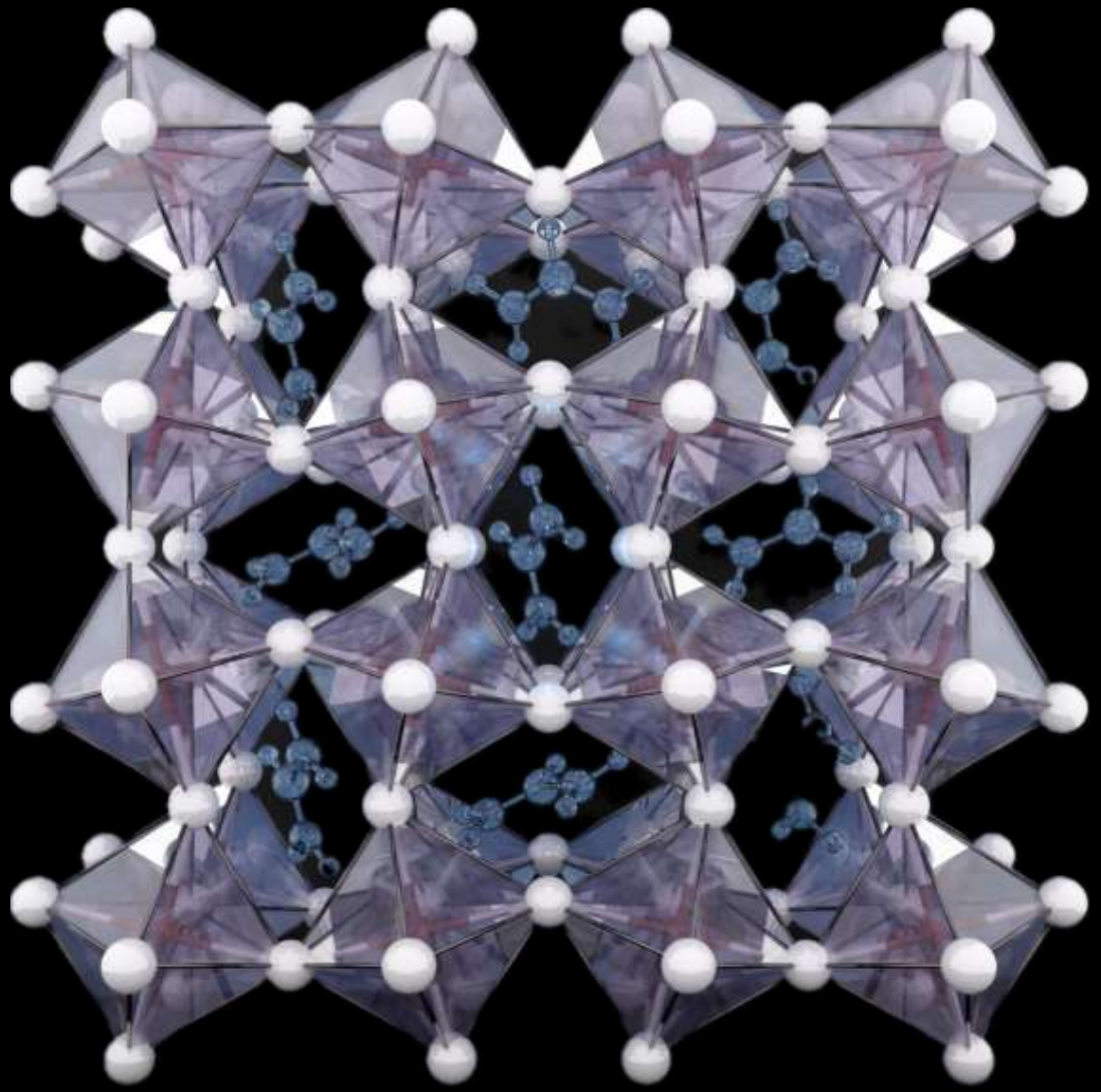

c-Si
$CH(NH_2)_2PbI_3$
Absorption coefficient (cm^{-1})
10^6
10^5
10^4
10^3
10^2
1.0
1.5
2.0
2.5
3.0
Photon energy (eV)



$CH(NH_2)_2PbI_3$ (formamidinium lead iodide-$FAPbI_3$)

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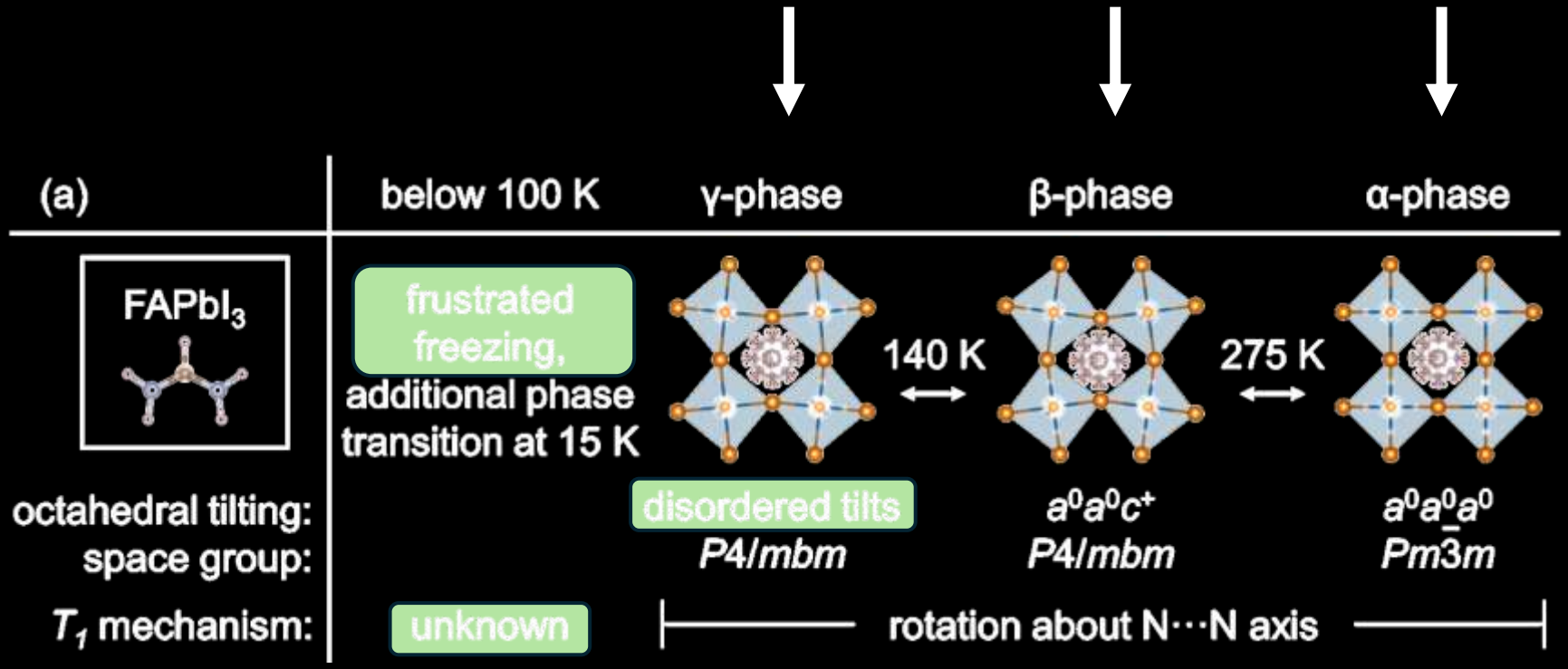
- One of many halide perovskites
- Sub-µm films absorb strongly
- Easy, low-temperature synthesis
- Efficiencies: single-junction ≥25% (lab); perovskite–Si tandems >33% (lab)
- Complex chemistry + strong dynamics → hard to model



D.H. Fabini et al., J. Am. Chem. Soc .139 (2017)

Low-temperature structure of $FAPbI_3$ unknown – needed to control and design $FAPbI_3$-based materials

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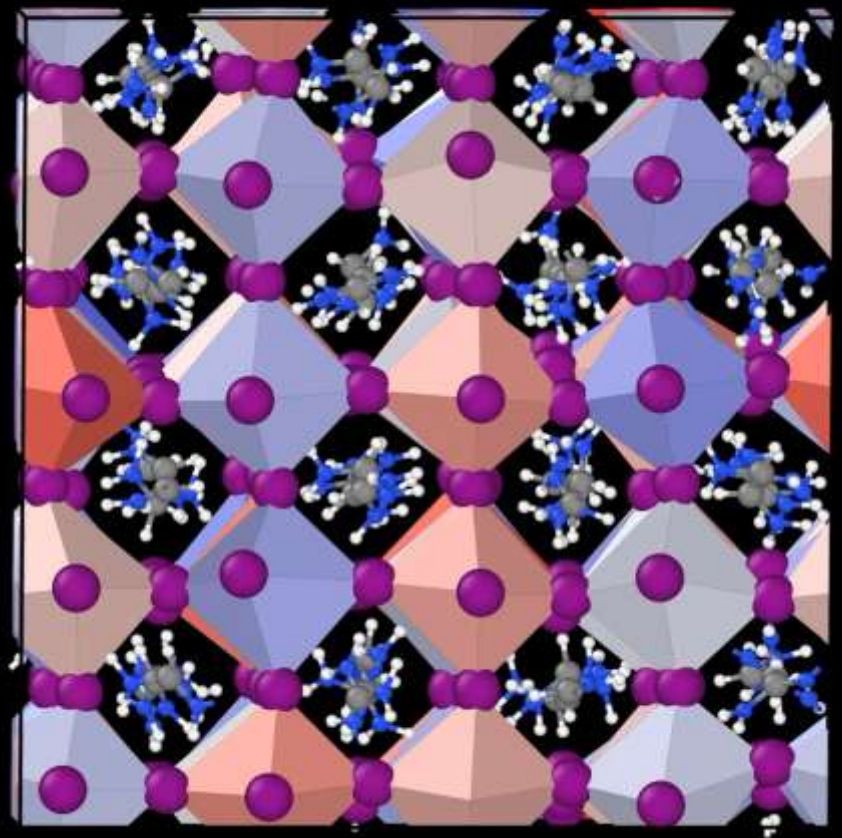
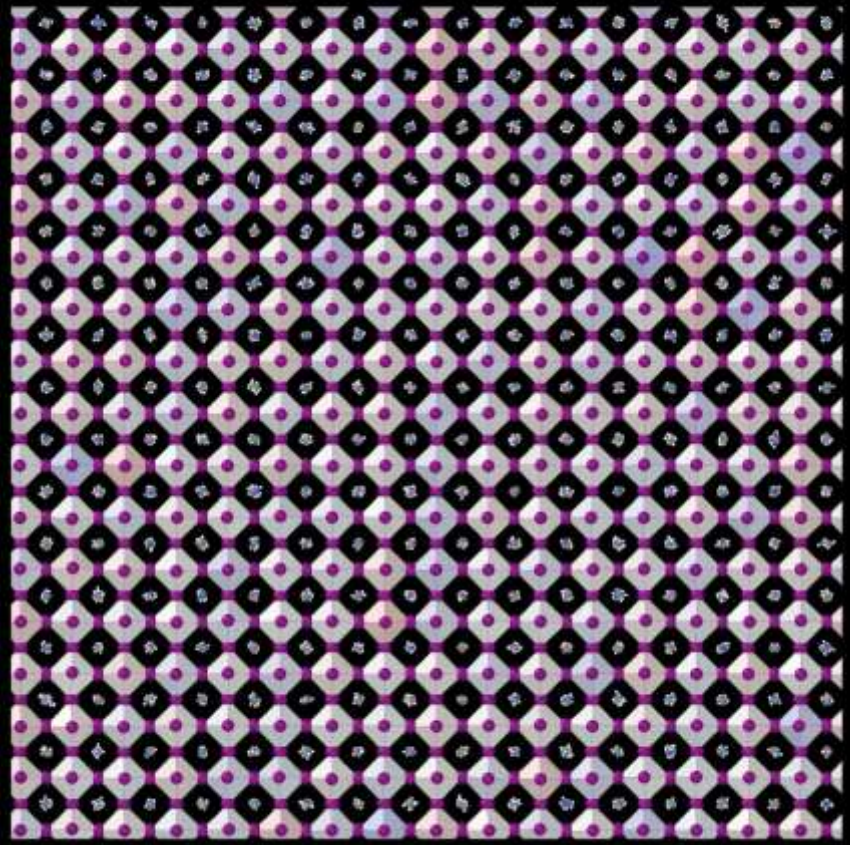
t=0.00 ps

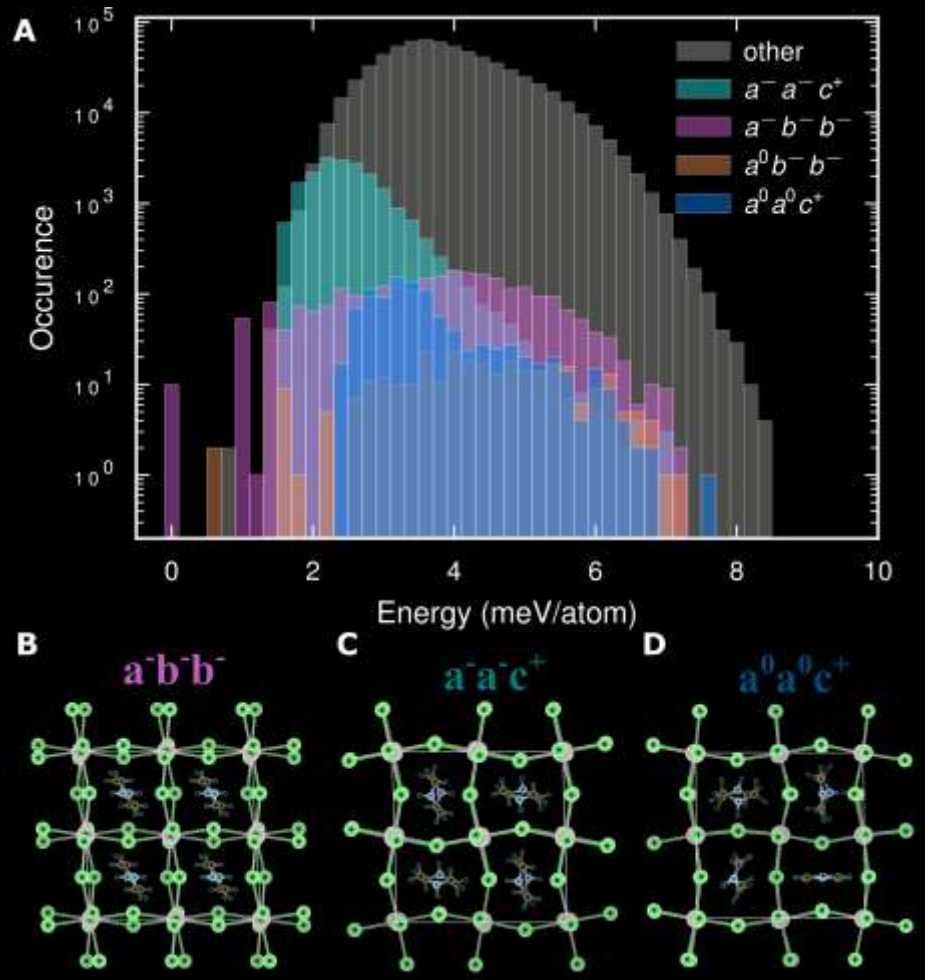


t=0 ps



Within a few years: **1000x** larger systems and **10000x** longer simulations thanks to ML and GPUs

Movies by Erik Fransson



Search among milion static structures with a neuroevolution (NEP) potential based

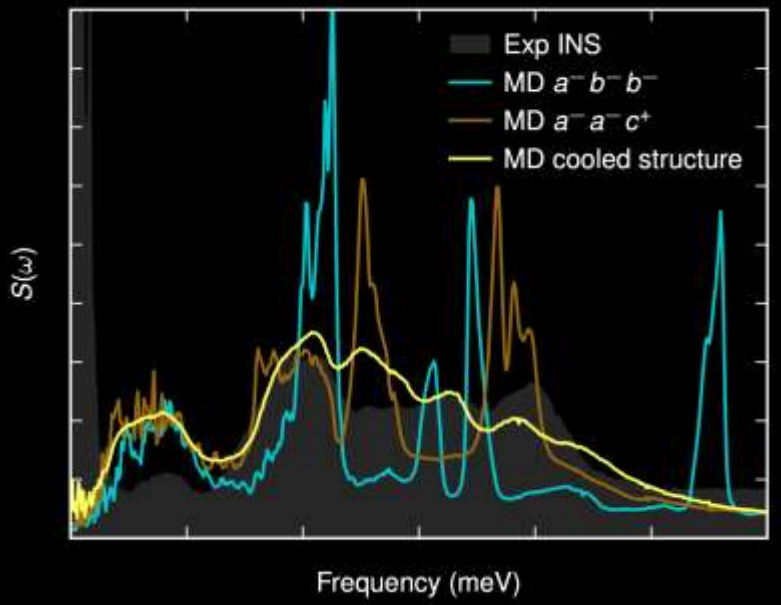
$a^-b^-b^-$ identified as ground state

Large-scale MD simulations show that structure “freezes” in a different structure, disordered **$a^-a^-c^+$**

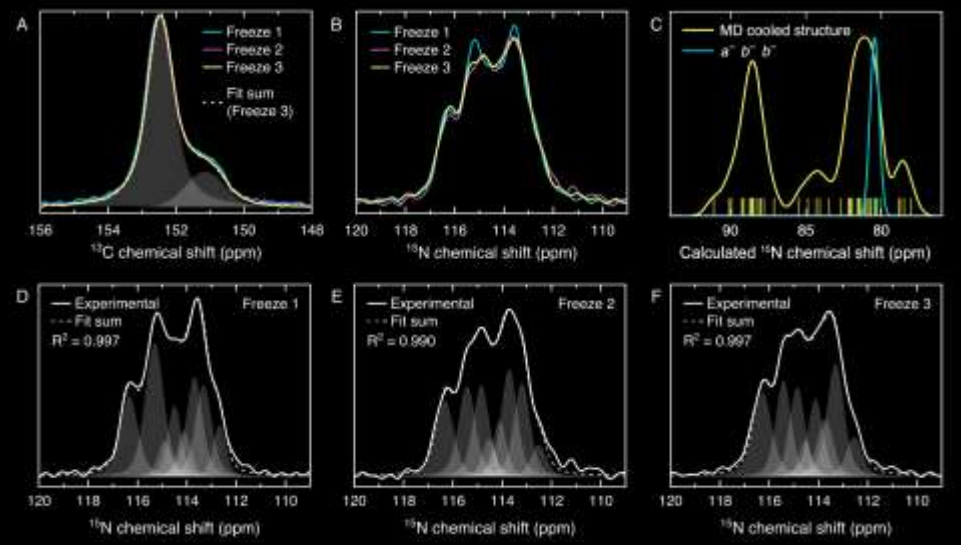
S Dutta, E Fransson, T Hainer, BM Gallant, DJ Kubicki, P Erhart, J Wiktor, *J. Am. Chem. Soc.* 2025, 147, 41, 37019

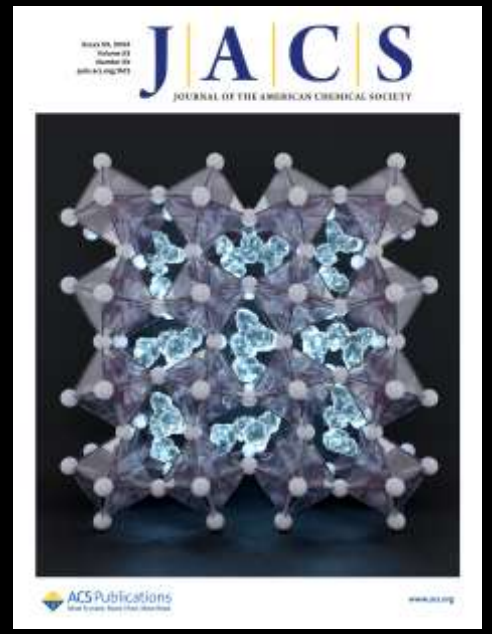
Comparison with experiment

Inelastic neutron scattering (INS)



Nuclear magnetic resonance (NMR)

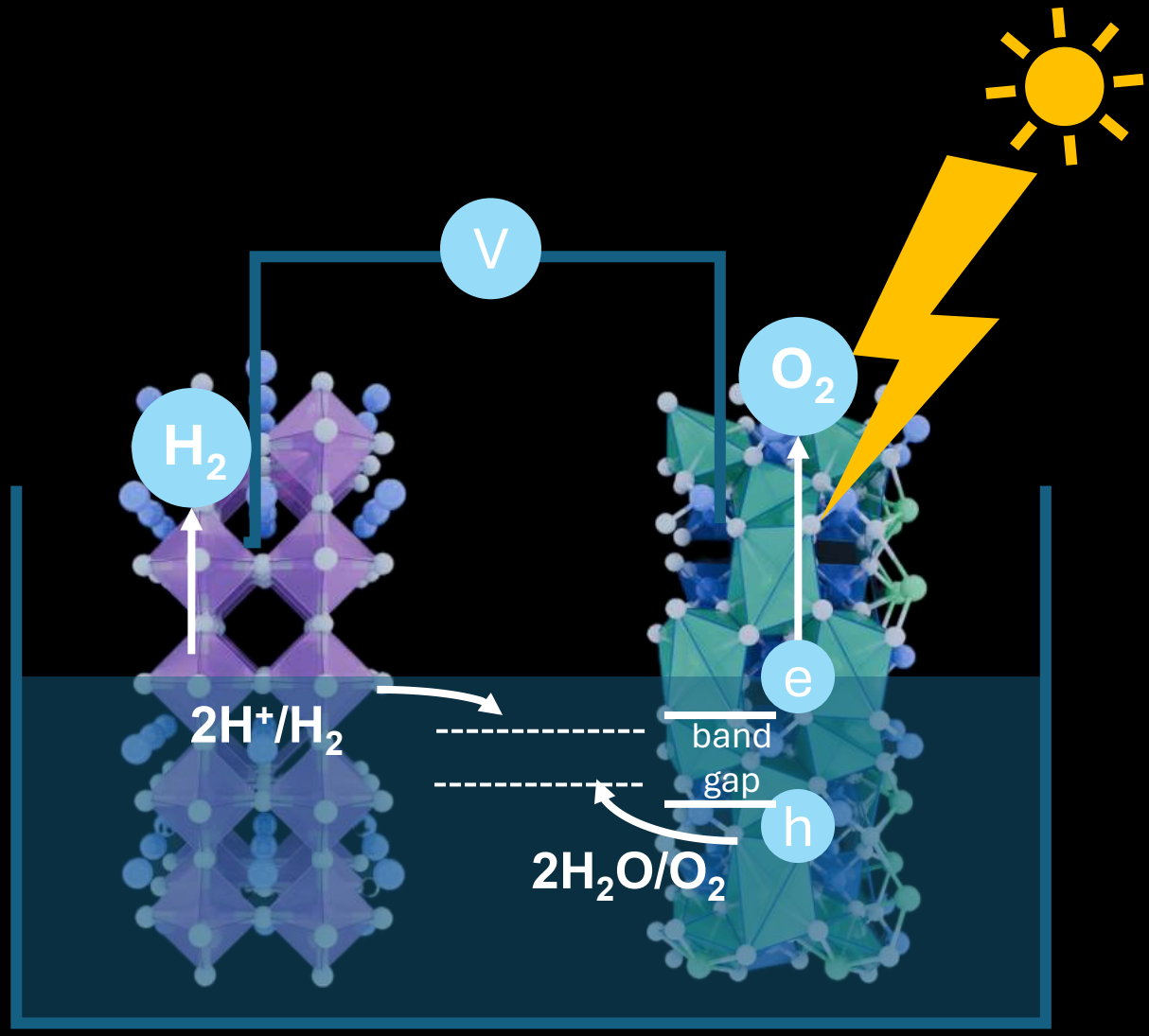




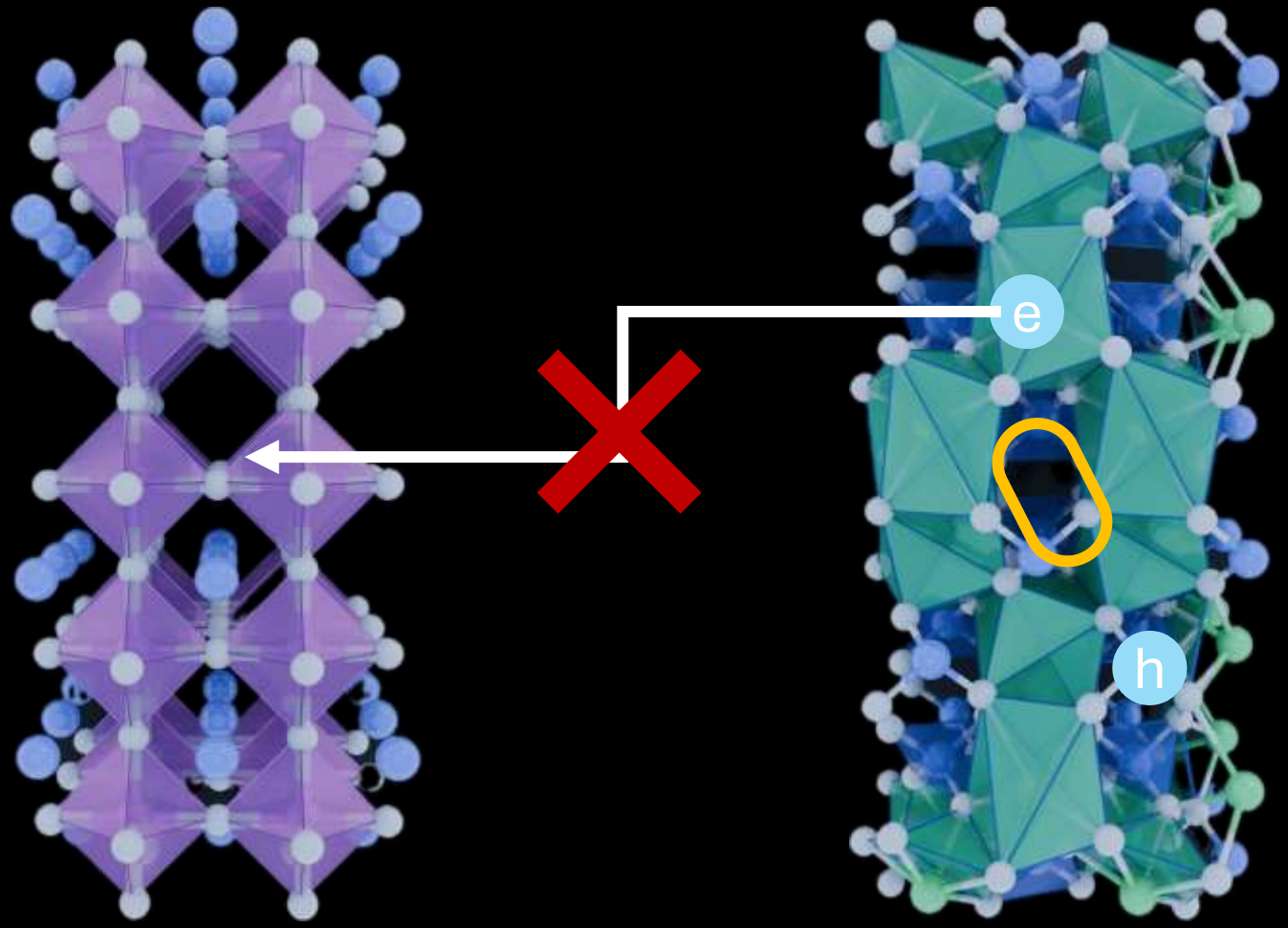
Our simulated “frozen” structure agrees with experiment

Water splitting

- Materials absorb light
- Extra charges created and separated
- H_2O separated into O_2 and H_2 (fuel)

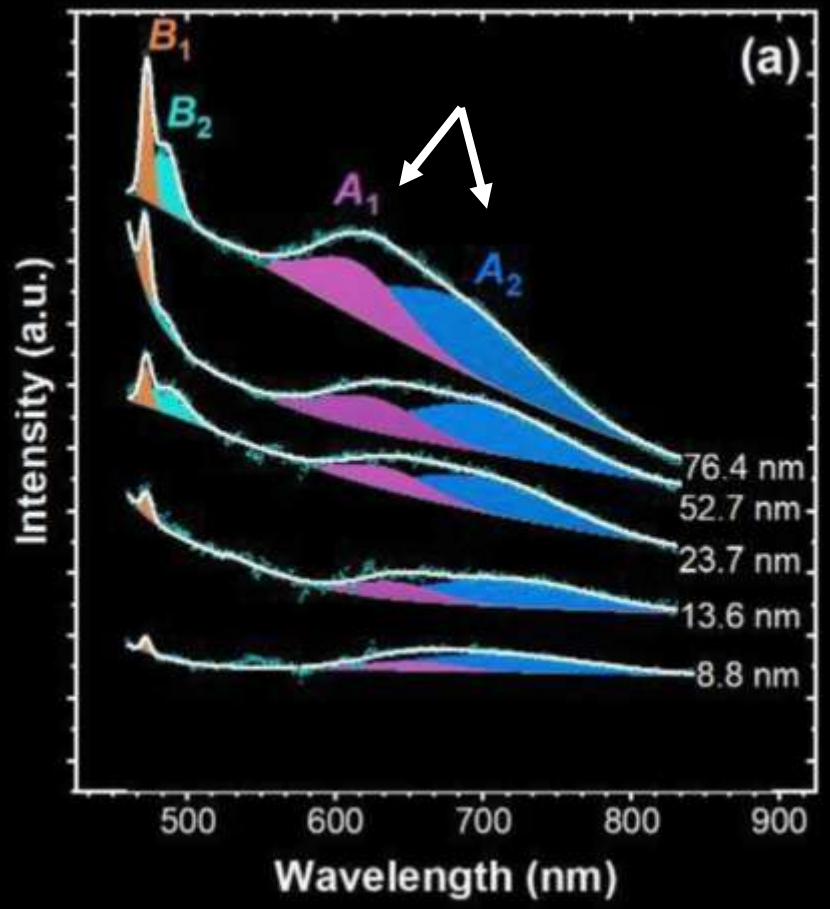


Charge trapping



Trapped charges cannot be used efficiently – we can predict if and how they form

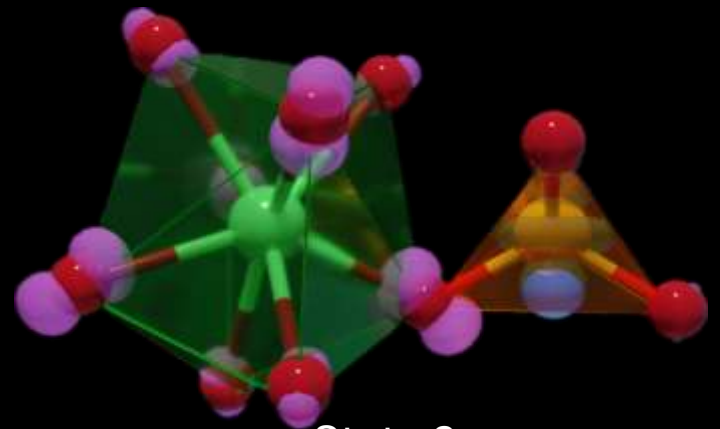
Self-trapped excitons – $BiVO_4$



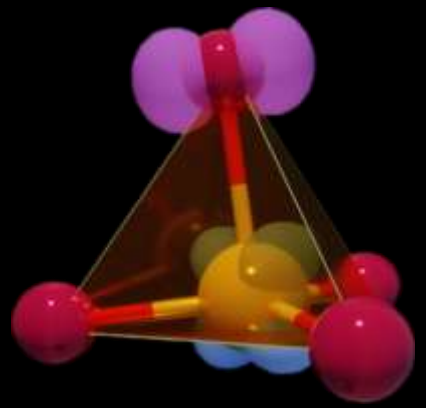
E. N. Fernandez, D. A. Grave, R. van de Krol, and F. F. Abdi, *Adv. Ener. Mater.* 13, no. 25 (2023): 2301075.

Photoluminescence measurements

State 1



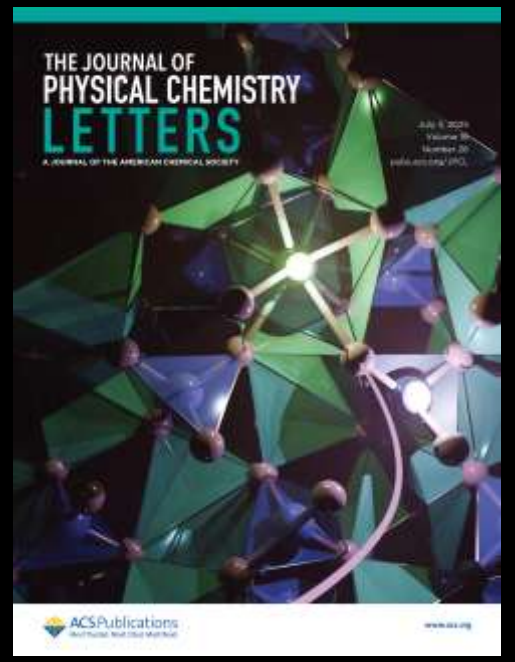
State 2



Two competing modes of trapping

T. Möslinger, N. Österbacka, and J. Wiktor, JPCL 16, 6861 (2025)

Requires hybrid density functional theory and time-dependent DFT calculations – **high-accuracy** but **time and memory consuming**



Summary

- Novel materials for solar application complex and challenging to model
- We found the low-temperature phase of $FAPbI_3$ combining DFT and ML
- Studying charge trapping requires advanced and expensive methods
- We can complement experiments in understanding materials

Acknowledgments

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NAISS

erc European Research Council