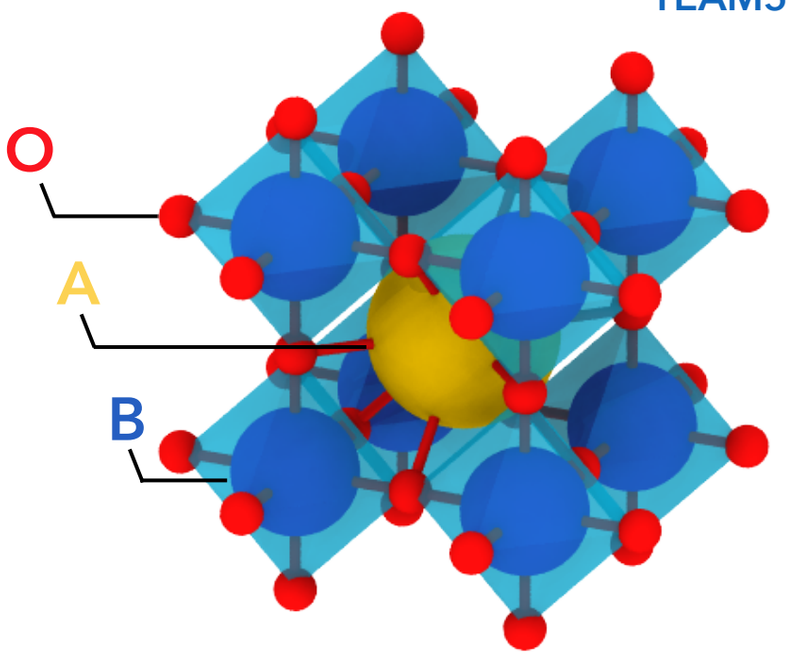
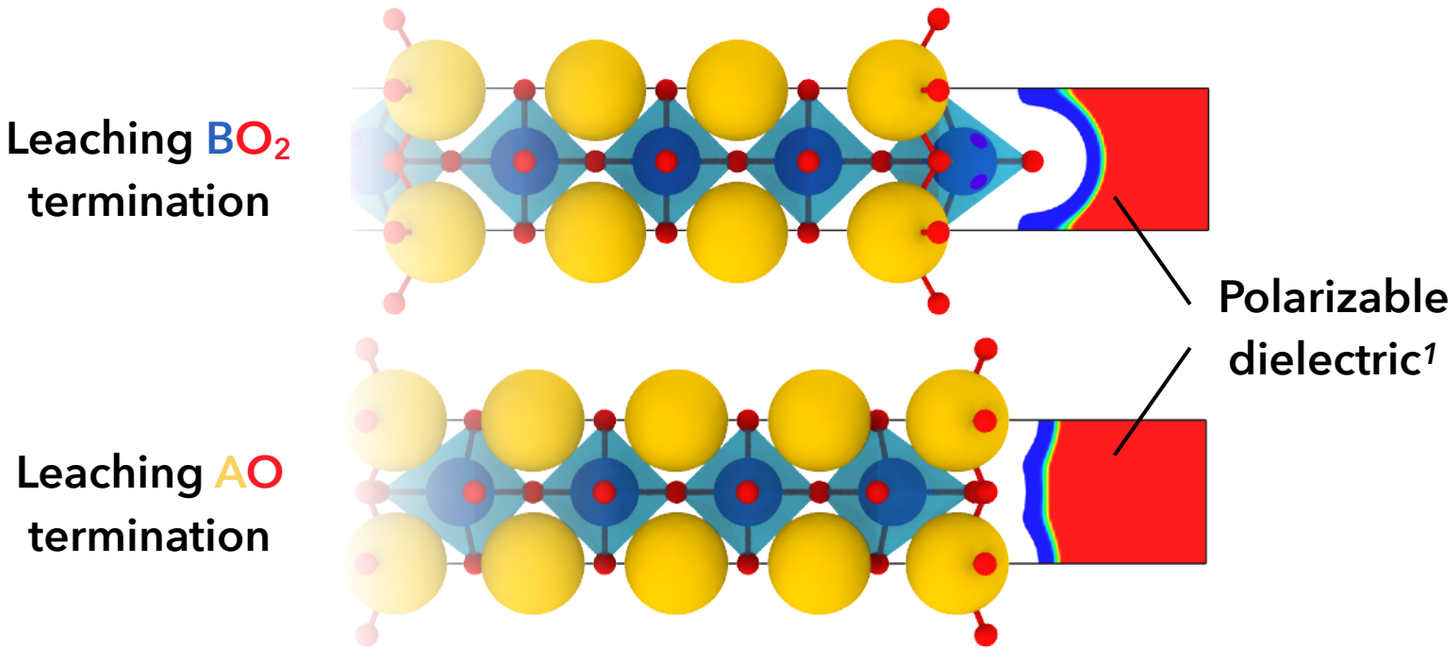
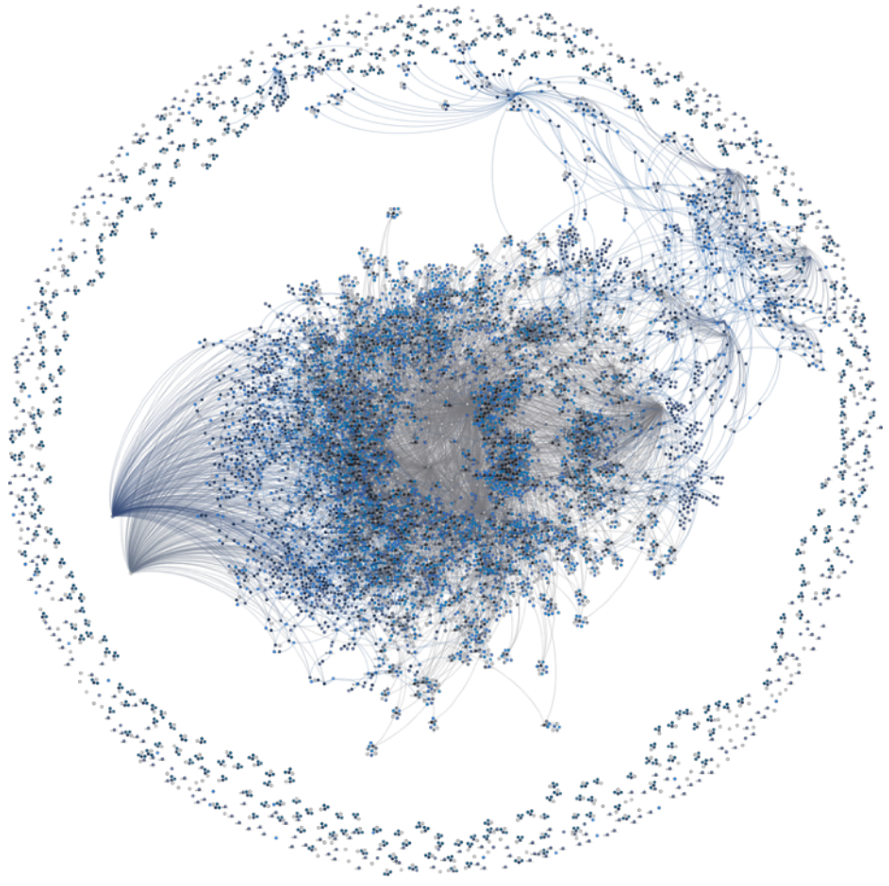
# MATDAT18: Predicting band edge positions of perovskite photocatalysts for water-splitting application

TEAM5: Yihuang Xiong, Weinan Chen, Wenbo Guo and Hua Wei
The Pennsylvania State University

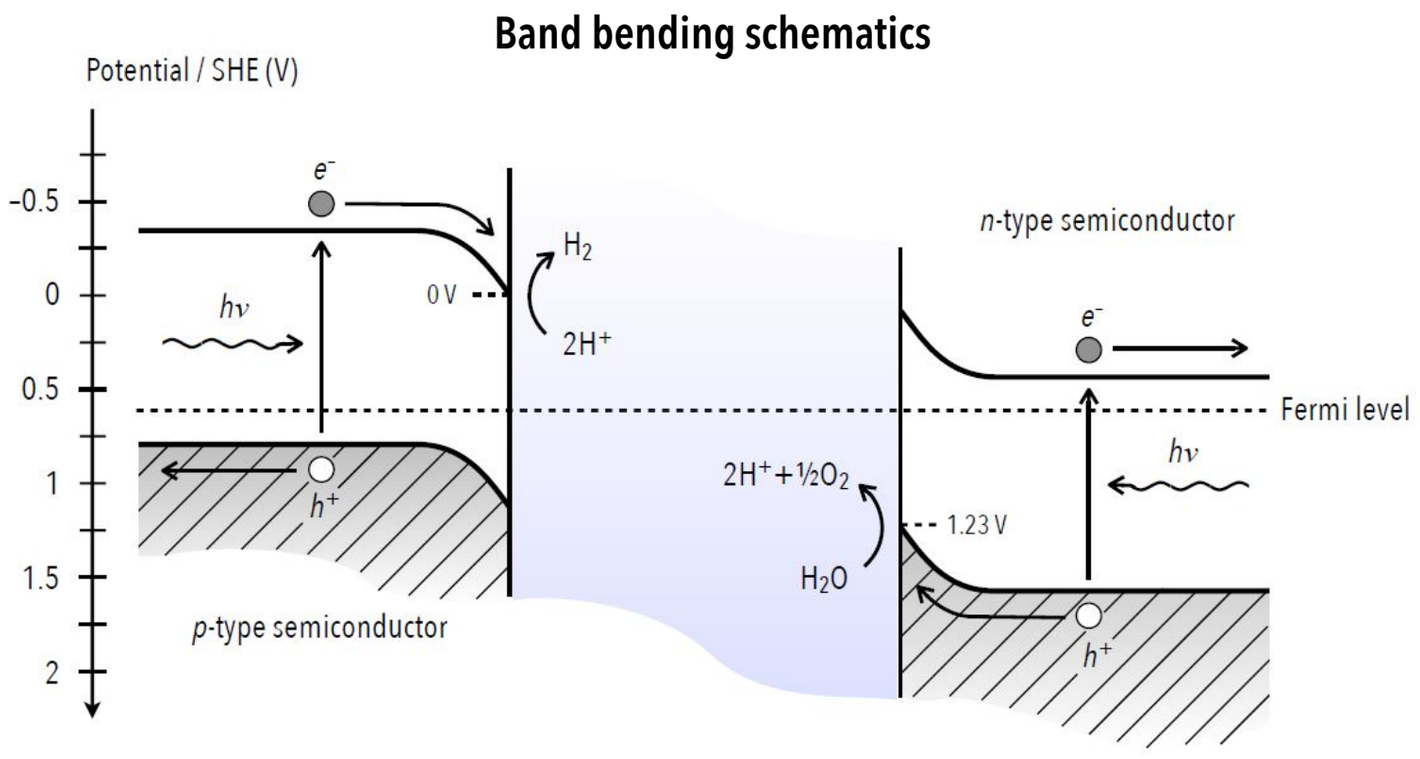



Cubic perovskite $ABO_3$



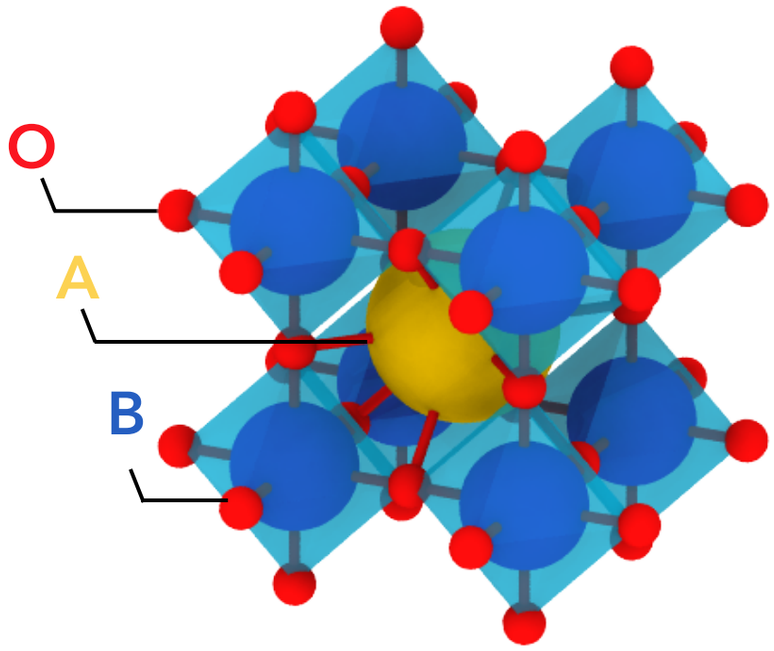



**Database structures of 328 perovskite slabs[2]**



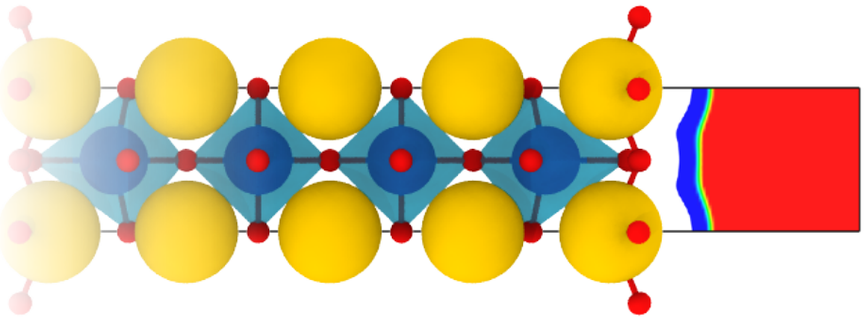

**1**.O. Andreussi, I. Dabo, and N. Marzari, *J. Chem. Phys.* **136**, 064102 (2012)
**2**.G. Pizzi, A. Cepellotti, R. Sabatini, N. Marzari, and B. Kozinsky, *Comp. Mat. Sci* **111**, 218-230 (2016)

# Predicting band edge positions and identify dominate descriptors

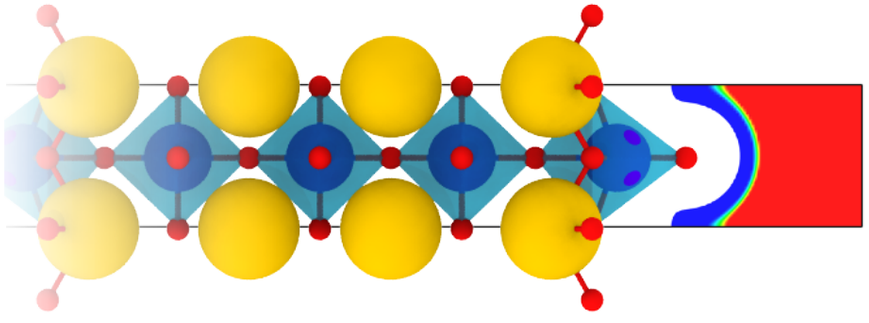



Cubic perovskite $ABO_3$

Leaching AO termination



Leaching $BO_2$ termination

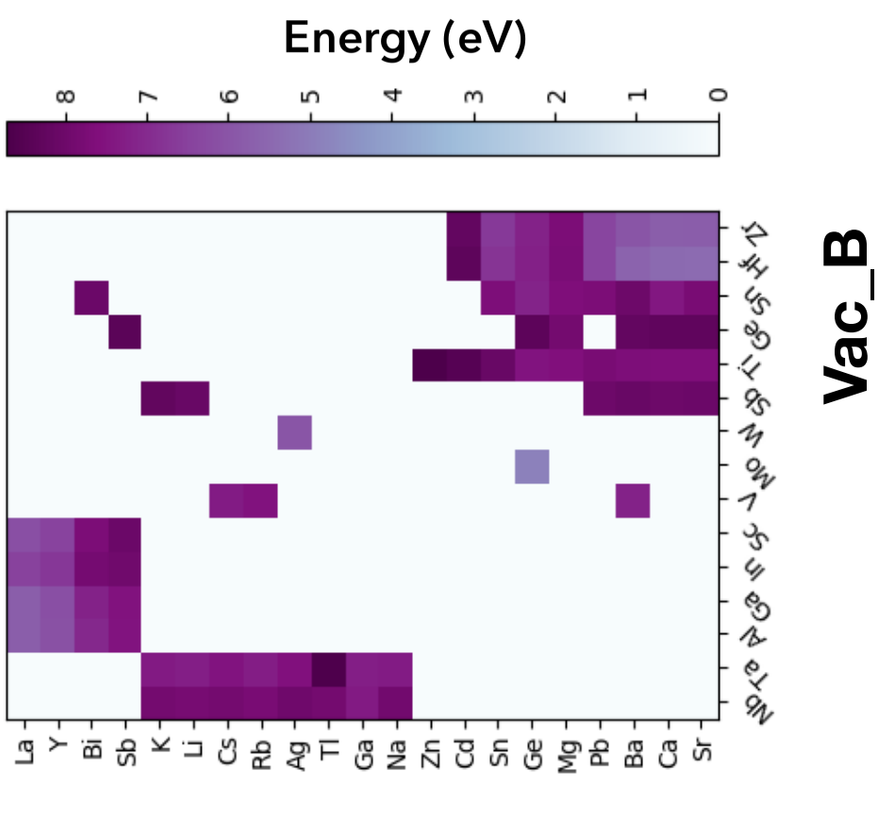


**Atomic descriptors**

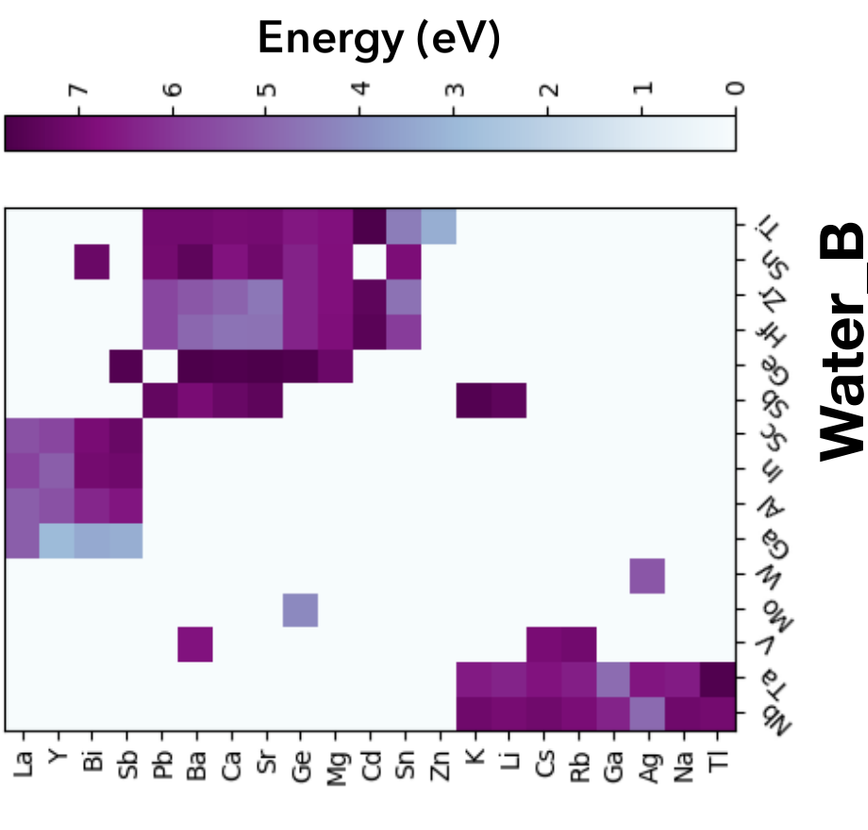
| | |
|---|---|
| Electronegativity | $\chi$ |
| Orbital radii | $s,\ p,\ d$ |
| Ionization potential | $I$ |
| Electron affiniity | $A$ |
| Solvation | $\mathcal{S}$ |

150 A-terminated slabs

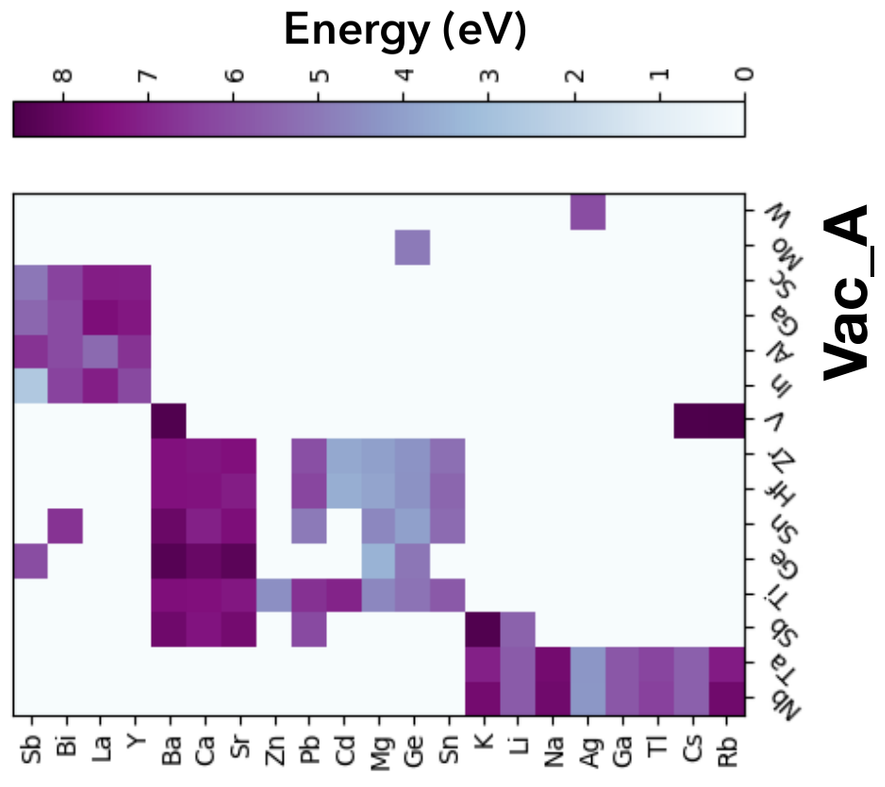
157 B-terminated slabs



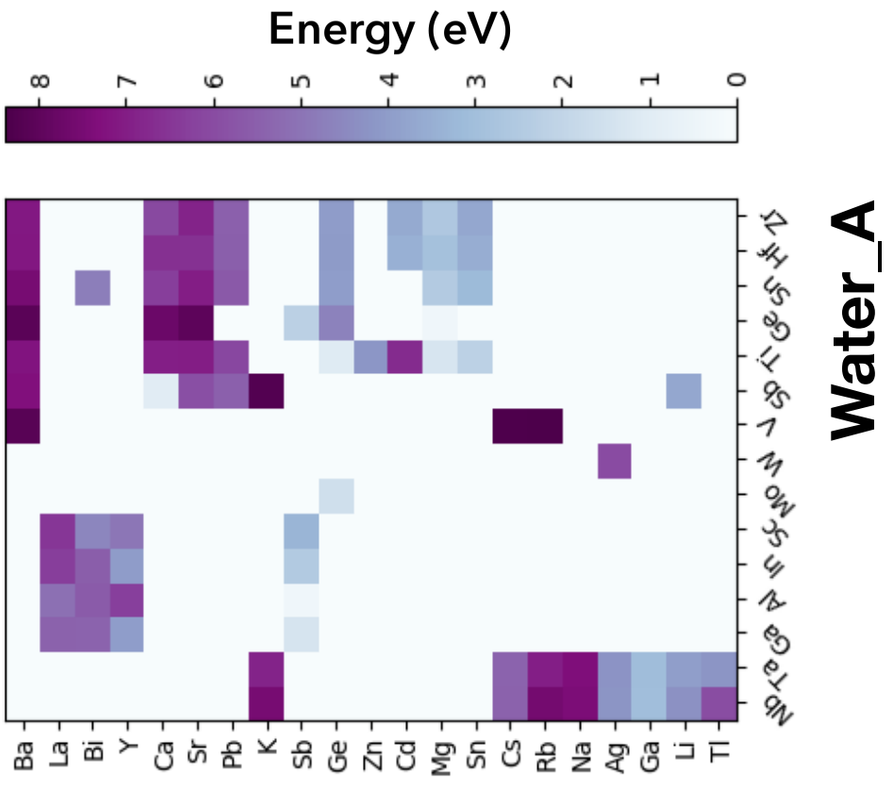

Vac_B




Water_B

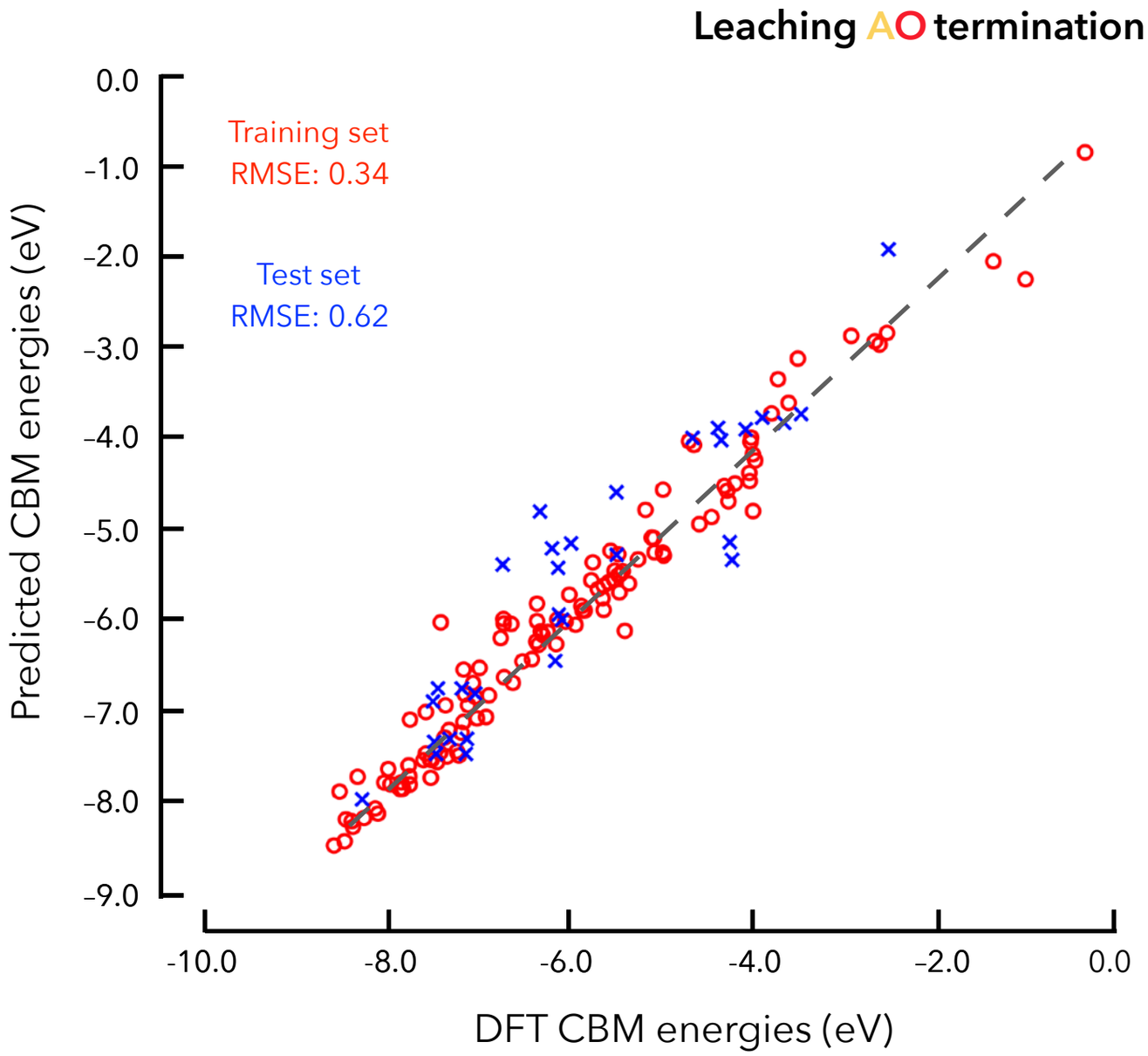


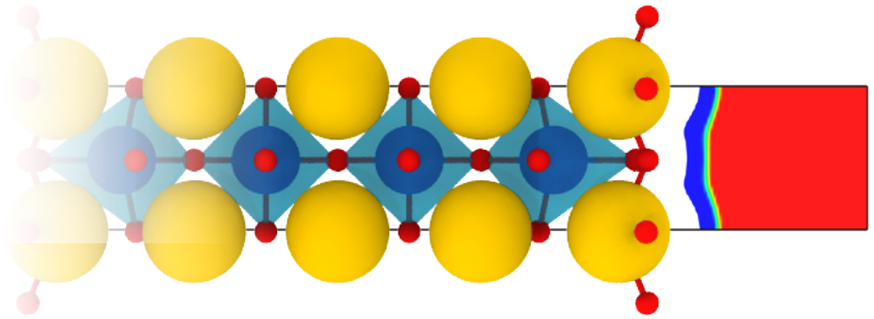

Vac_A




Water_A

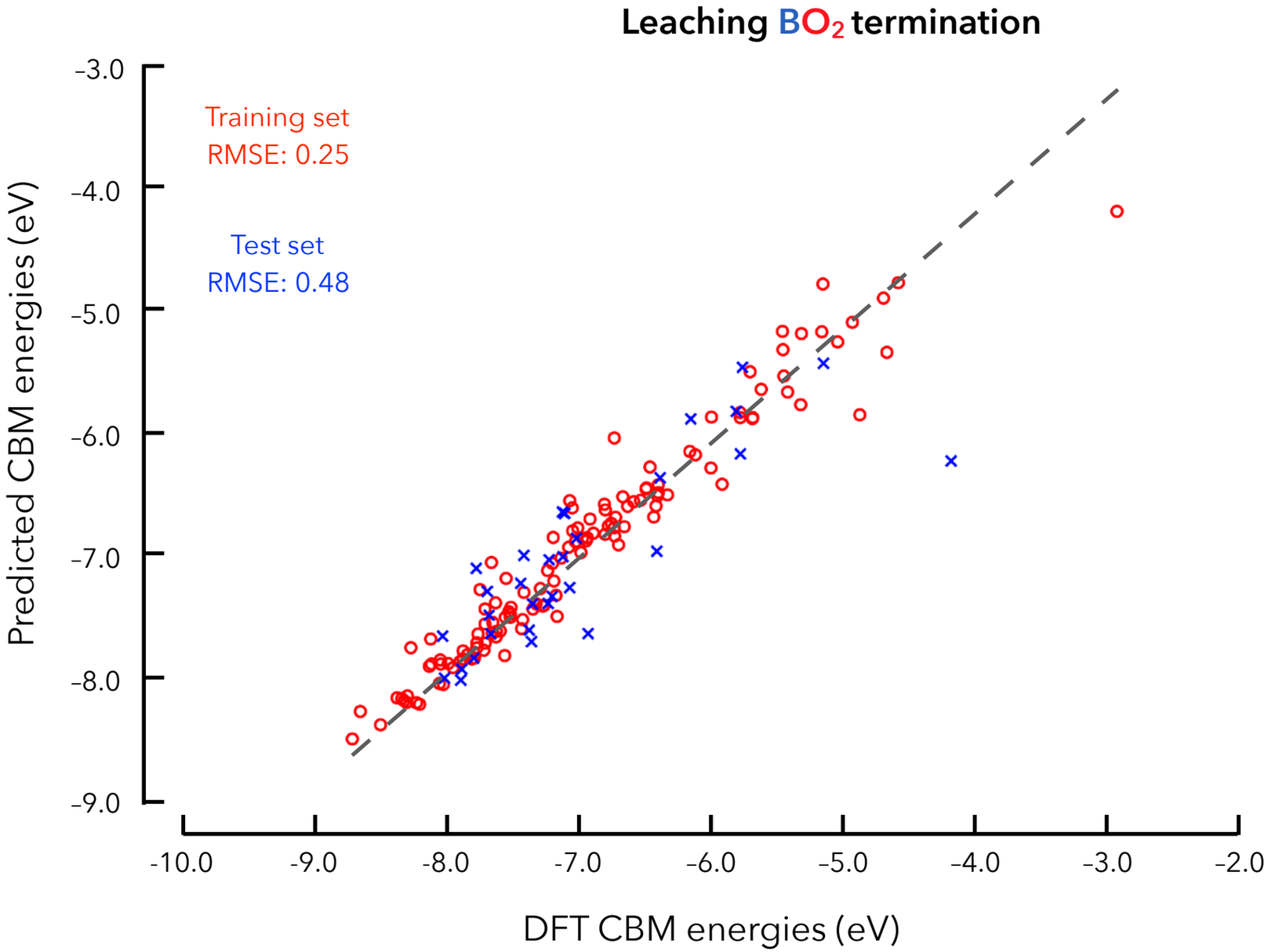
# Random forests model performance

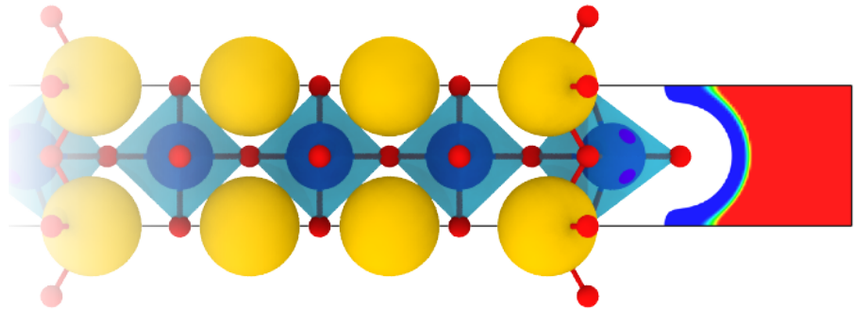


| Descriptor | Weight |
|---|---|
| $A_I$ | 21% |
| $A\chi$ | 18% |
| $A(s)$ | 15% |
| $A(d)$ | 11% |
| $\mathcal{S}$ | 7% |

# Random forests model performance cont.



| Descriptor | Weight |
|---|---|
| $\mathcal{S}$ | 19% |
| $B_I$ | 15% |
| $A(d)$ | 15% |
| $B\chi$ | 14% |
| $B_A$ | 9% |