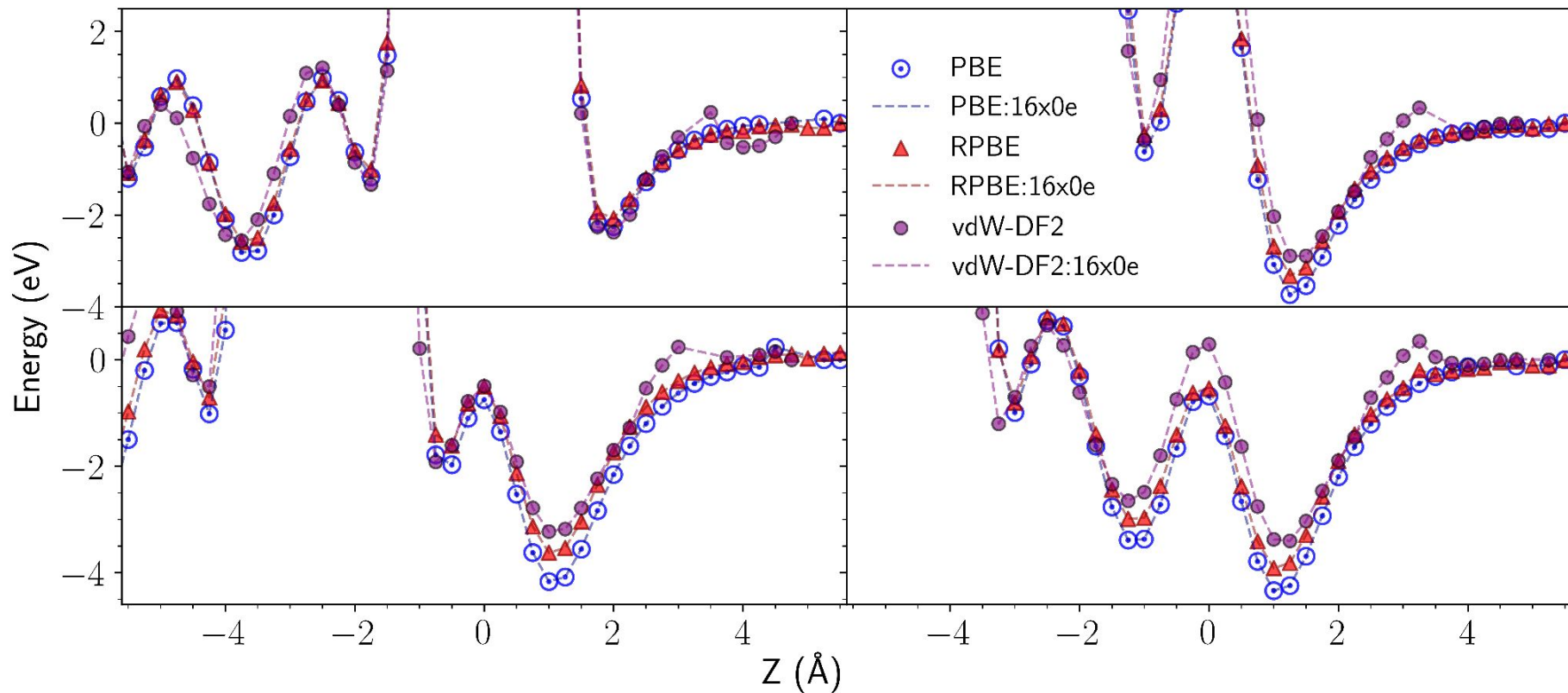
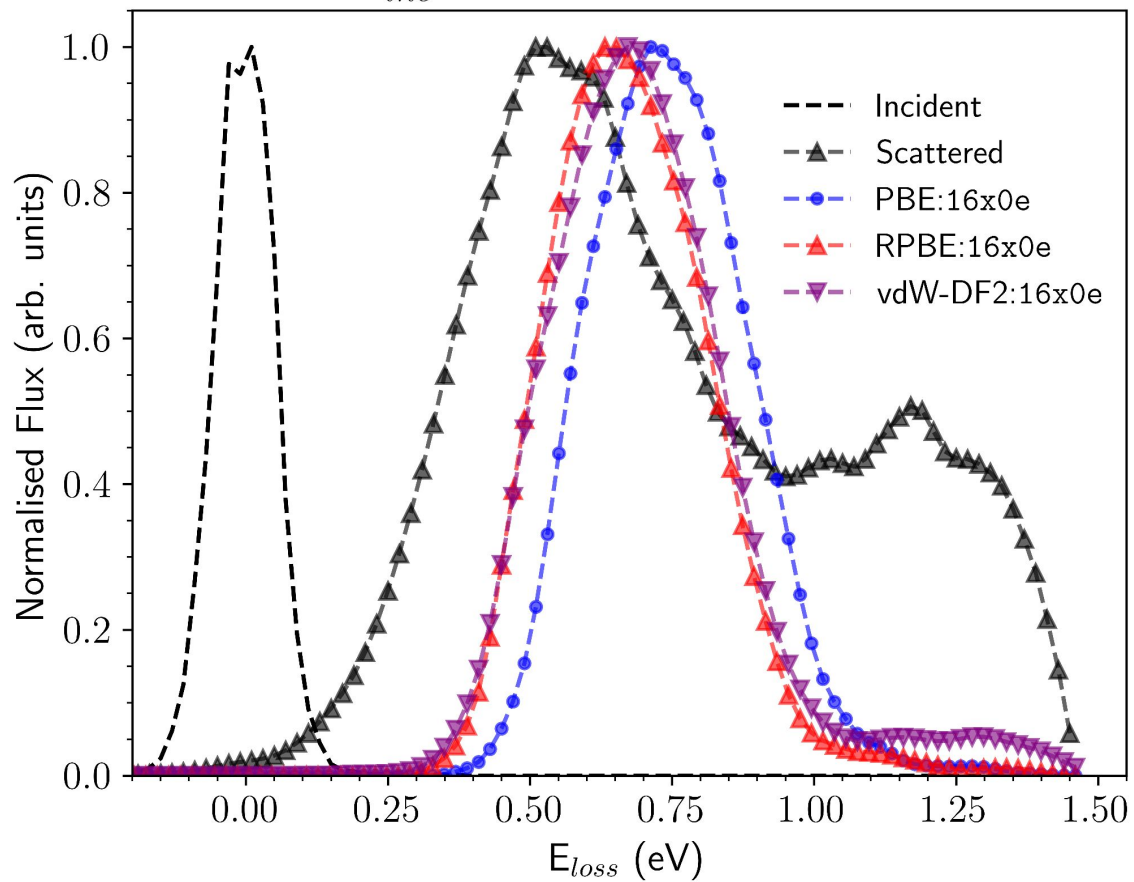


C Atom Scattering

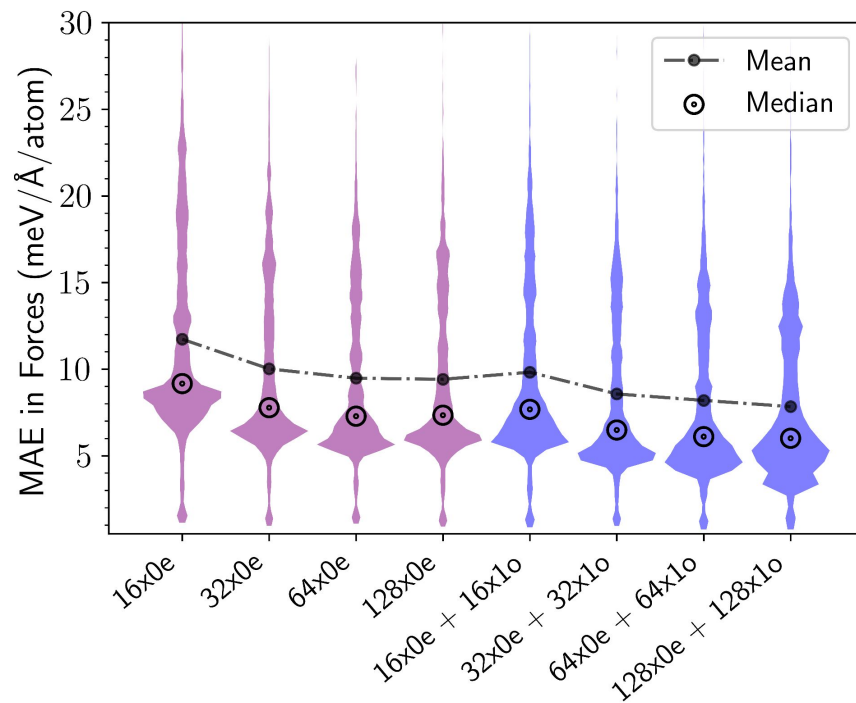
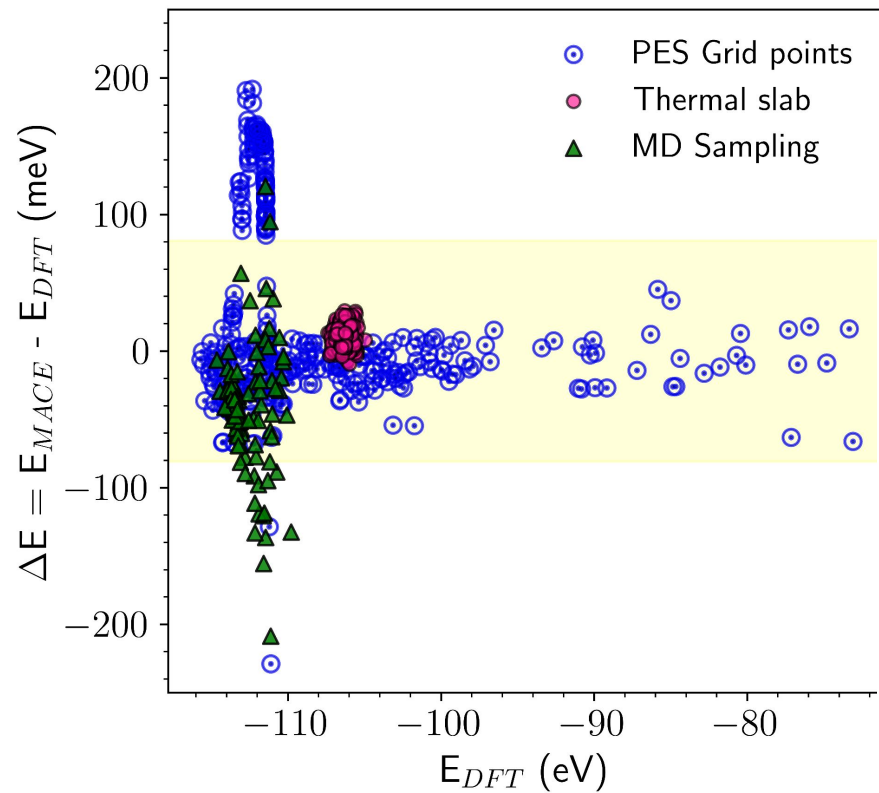
PES Grids for high symmetry sites



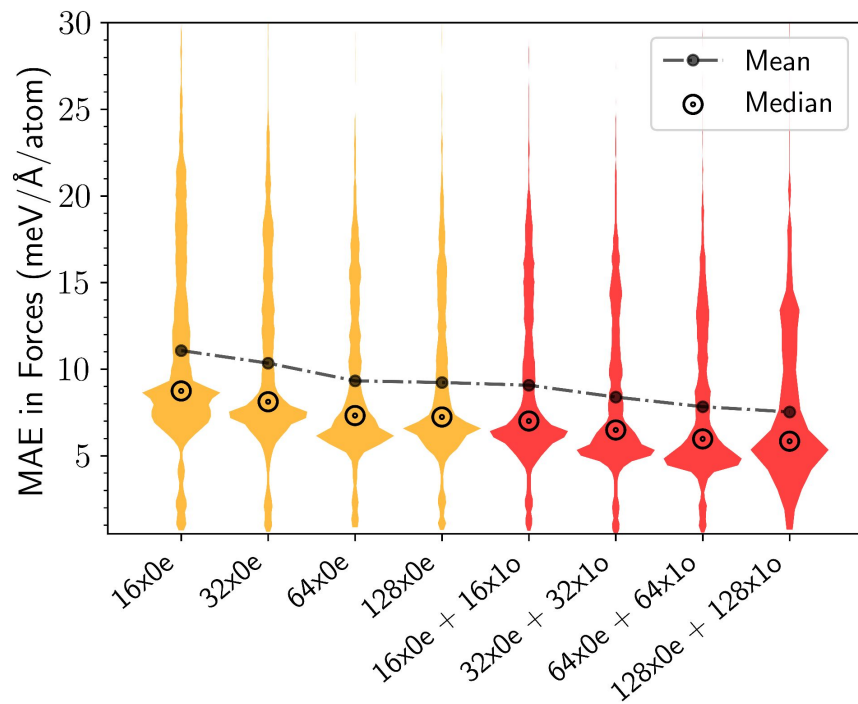
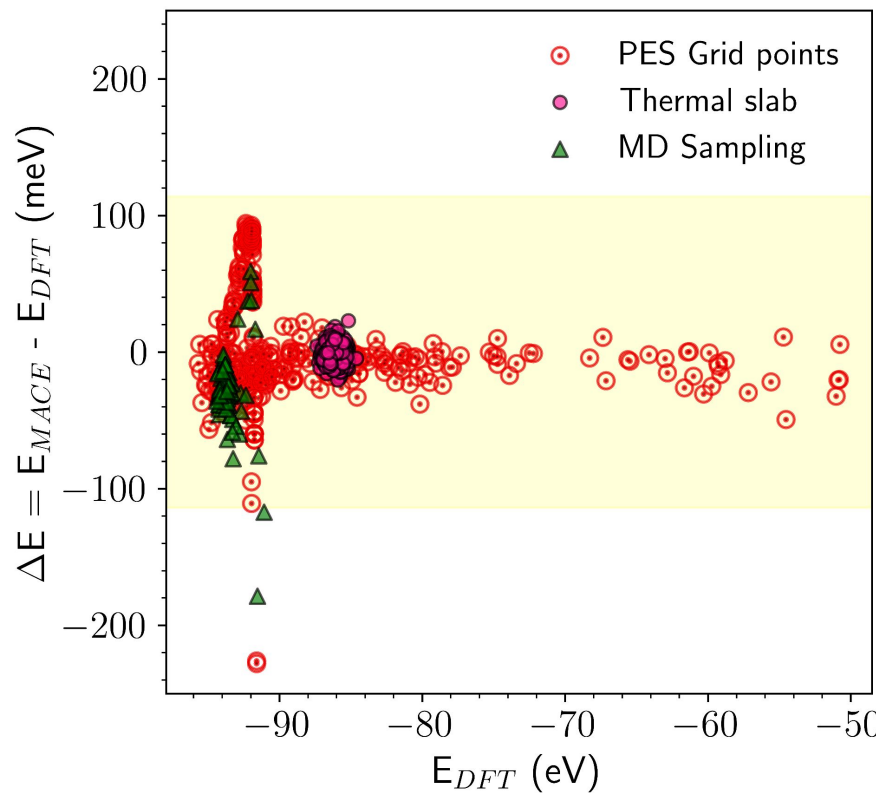
$$E_{inc} = 1.46 \text{ eV and } \Theta = 0^\circ$$



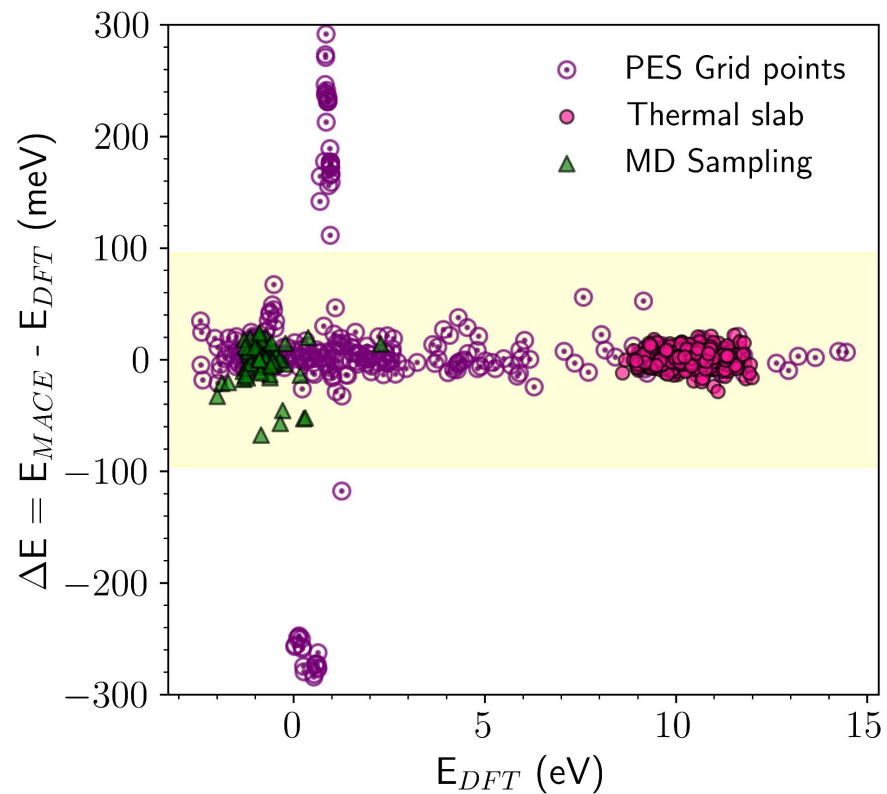
PBE: 16x0e



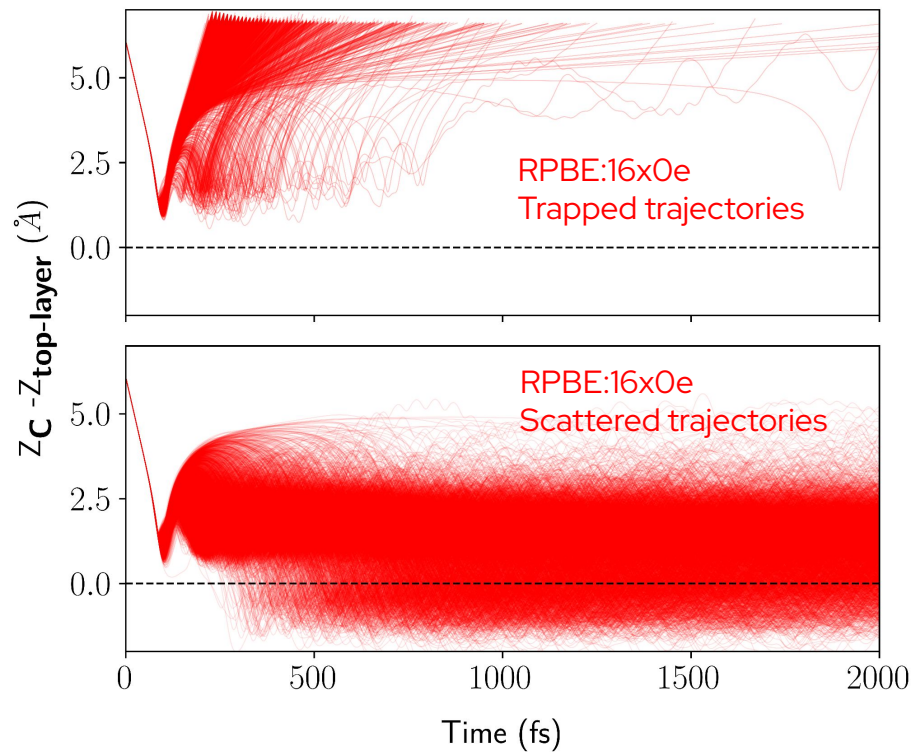
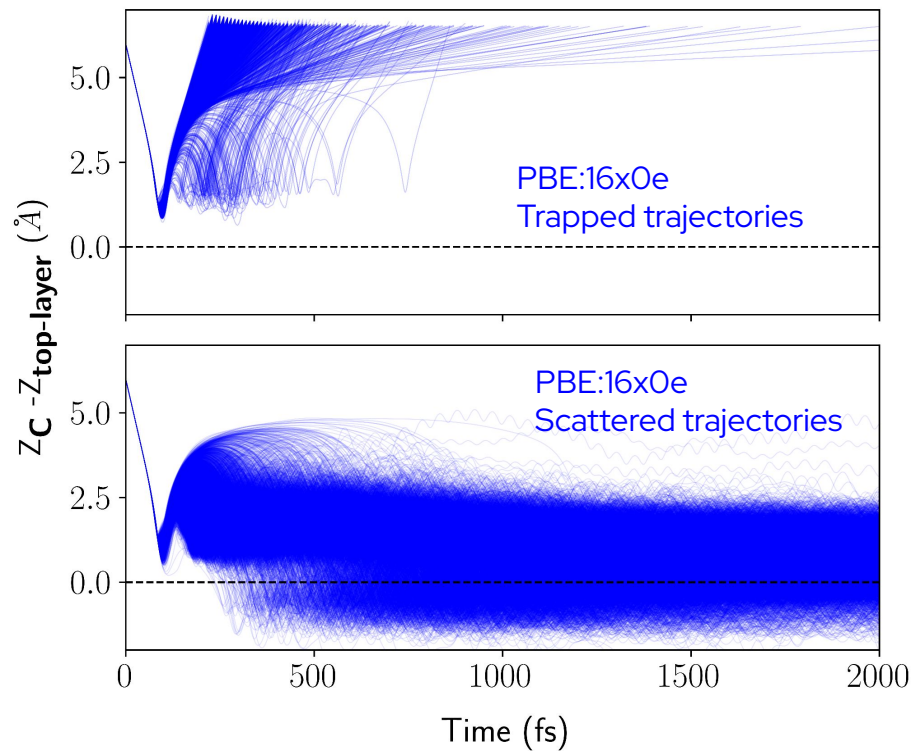
RPBE: 16x0e

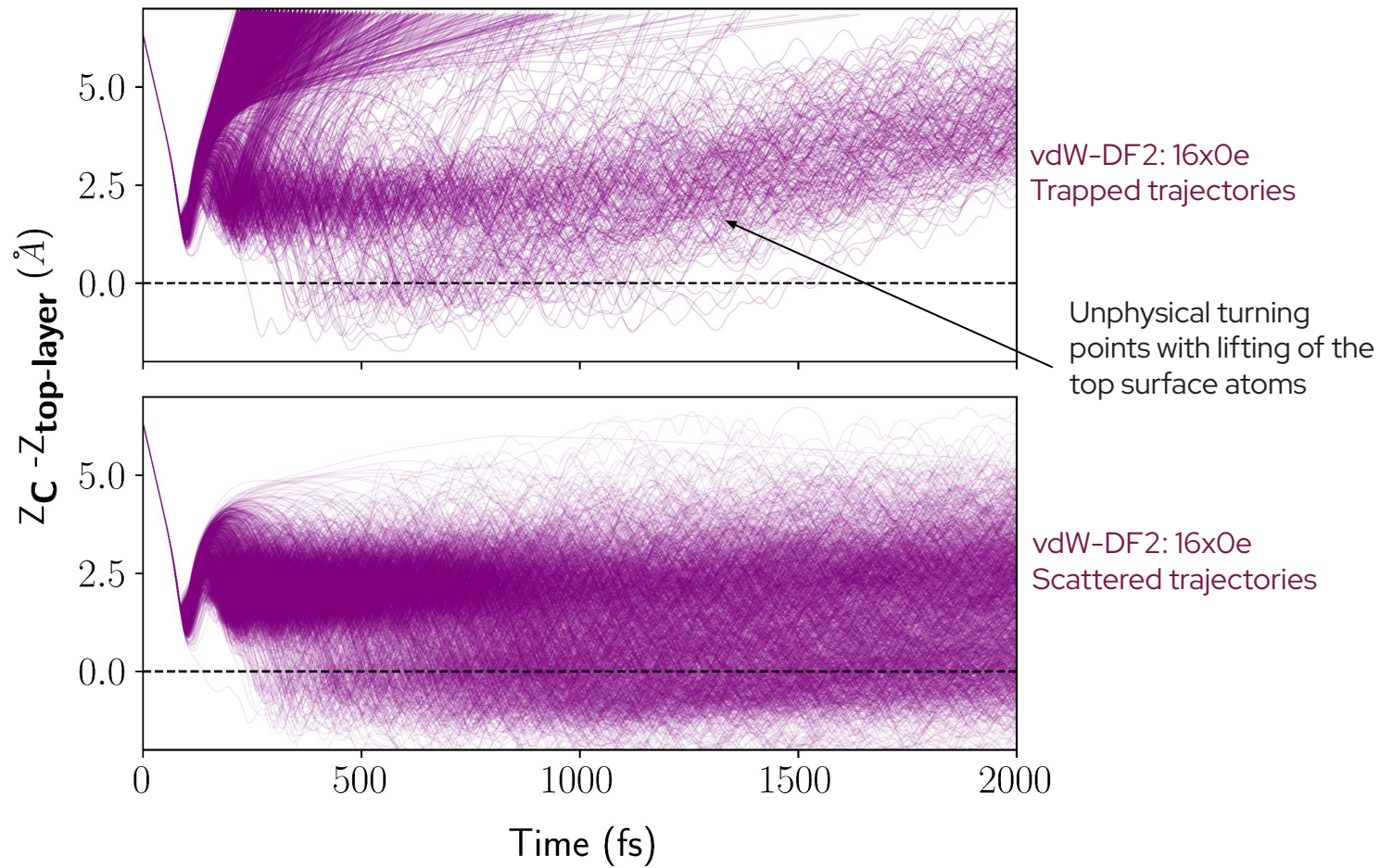


vdW-DF2:16x0e



10k Scattering Trajectories in a snapshot

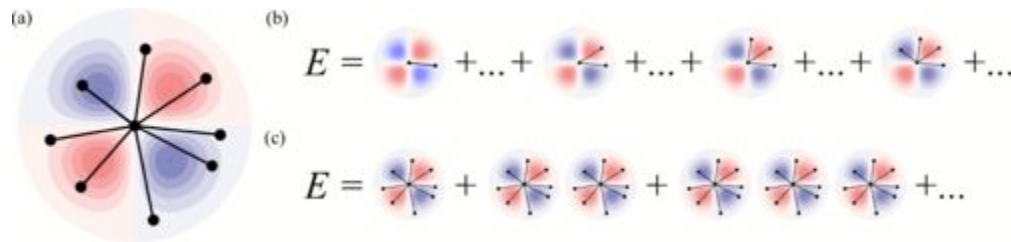




Machine-Learned Interatomic Potentials (MLIPs)

MACE is equivariant message passing neural network (MPNN) model that utilizes the atomic-cluster expansion (ACE) framework to pass higher body-order messages. In our models, we have only used upto 3-body features.

$$E = V_0 + \sum_i V^{(1)}(\mathbf{r}_i) + \frac{1}{2} \sum_{ij} V^{(2)}(\mathbf{r}_i, \mathbf{r}_j) + \frac{1}{3!} \sum_{ijk} V^{(3)}(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) + \frac{1}{4!} \sum_{ijkl} V^{(4)}(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k, \mathbf{r}_l) + \dots,$$



To generate the DFT dataset to train MLIP models, convergence tests were performed for a 3x3x4 slab of Au(111) and, a k-mesh of 15x15x1 with sigma=0.2 eV was used for all the calculations.

DFT	Total # of configurations	Symmetry sites	Randomly Sampled	Thermalised Slab
PBE	1225	455	483	500
RPBE	1236	475	495	495

Models (Hidden irreps)	Total number of parameters
16x0e	31808
16x0e + 16x1o	41856
32x0e	51440
32x0e + 32x1o	78576

Almost all the models that were trained had :

RMSE in Energy: ~1.8 meV / atom

RMSE in Forces: ~ 15 meV / Å / atom

Drautz, Ralf. Physical Review B 99.1 (2019): 014104.

Batatia, Ilyes, et al. Advances in neural information processing systems 35 (2022): 11423-11436.

Stark, Wojciech G., et al. Machine Learning: Science and Technology 5.3 (2024): 030501.