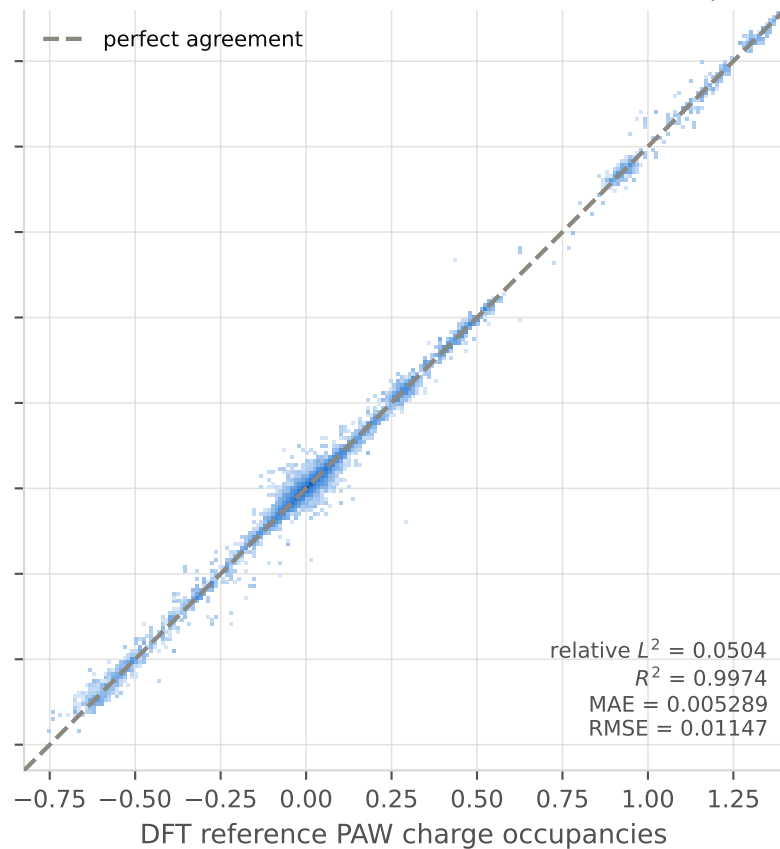
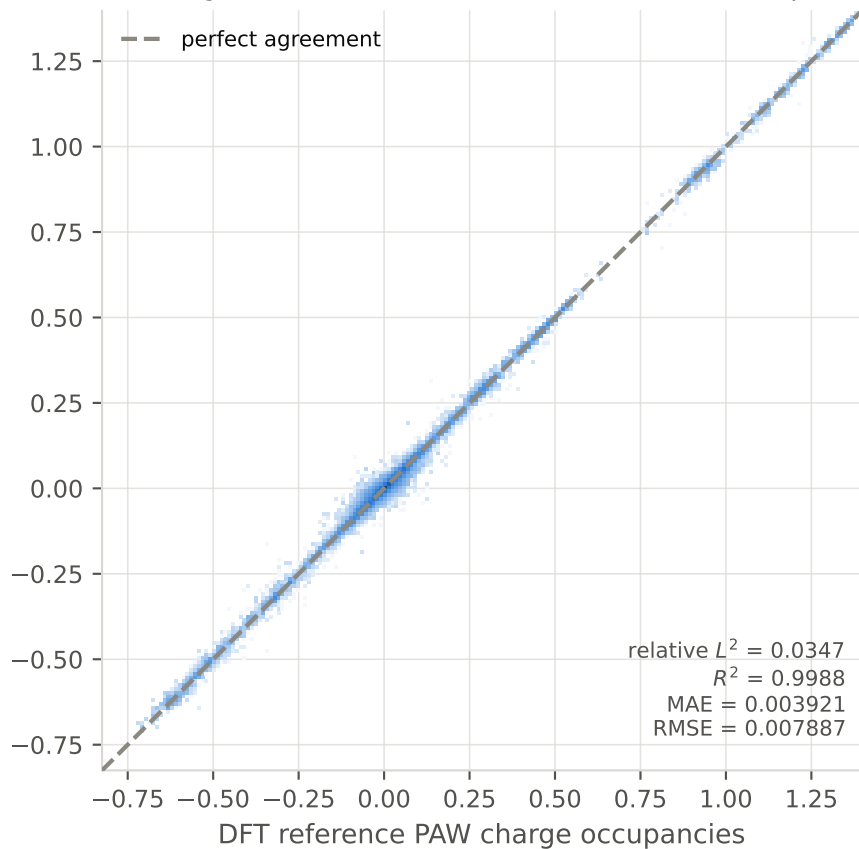


Parity over every structure: PAW charge occupancies

training set — 303 structures, 241,149 voxels sampled

validation set — 88 structures, 77,394 voxels sampled

FNO prediction PAW charge occupancies



share of the split's sampled voxels per bin