Supplementary Information – Nuclear Quantum Effects of Surface Mediated C-H Activation

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Machine learning interatomic potential training

Training Error

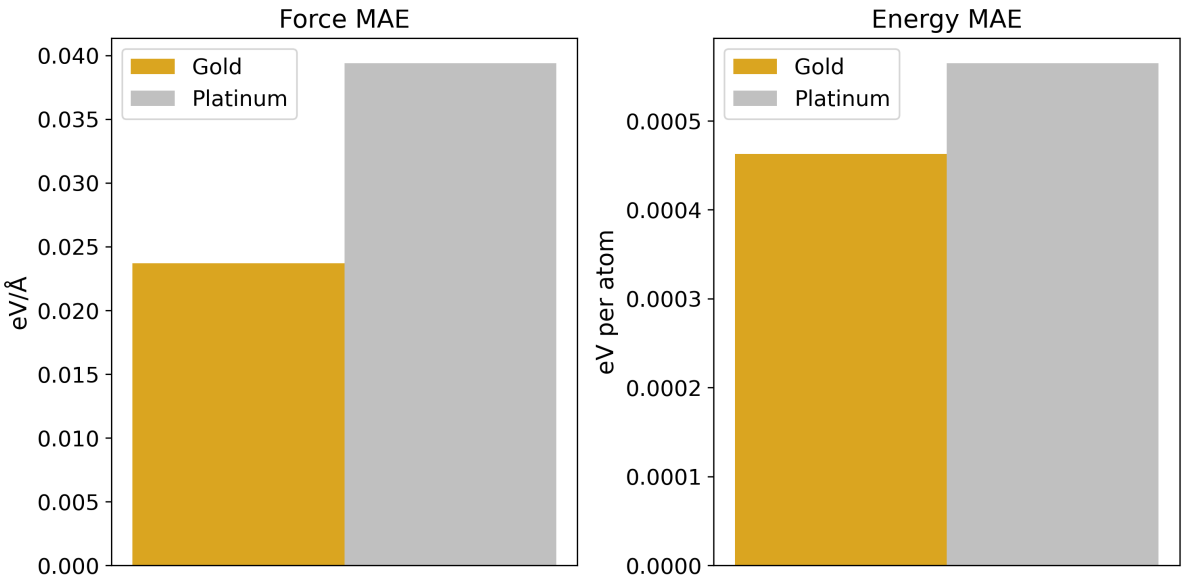

Figure S1: Training error of the potentials. The validation set MAE for the Au potential is 0.000475 eV/atom and 0.0243 eV/Åfor the energy and forces, respectively. The validation set MAE for the Pt potential is = 0.000583 eV/atom and 0.0417 eV/Åfor the energy and forces, respectively.

Parity Plot

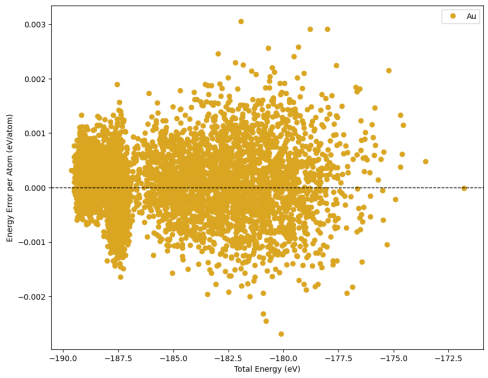

Figure S2: Training energy error per atom for the Au(111) dataset.

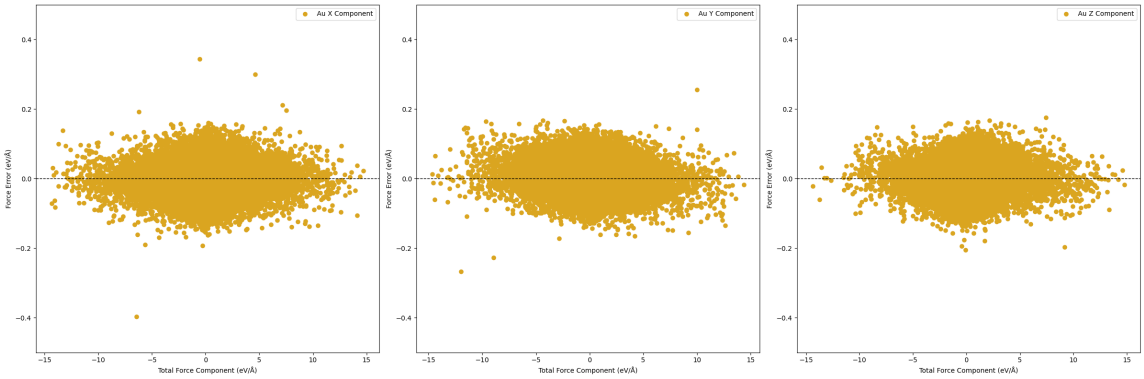

Figure S3: Training force component error for the Au(111) dataset.

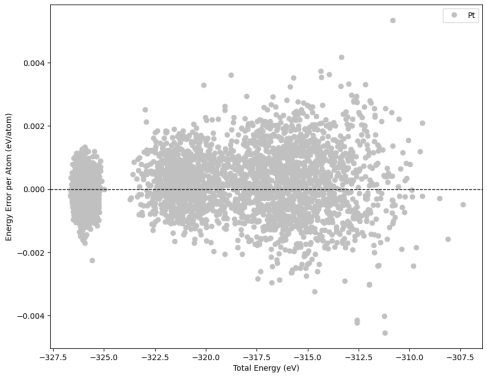

Figure S4: Training energy error per atom for the Pt(111) dataset.

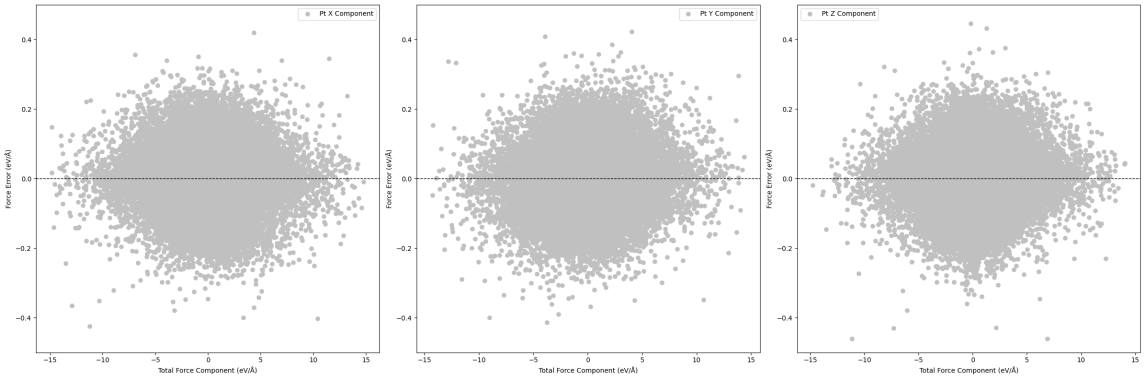

Figure S5: Training force component error for the Pt(111) dataset.

Bead convergence of centroid molecular dynamics

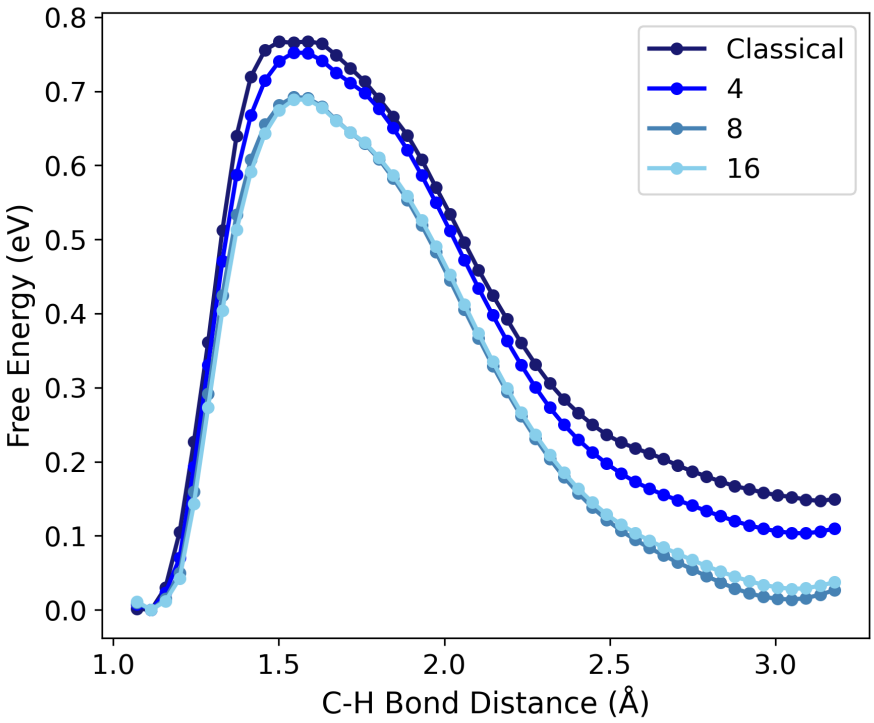

Figure S6: Bead convergence test of the centroid molecular dynamics derived potential mean force for CH_3 activation on Pt(111).