Supporting Information:

Machine Learned Corrections to Mean-Field Microkinetic Models at the Fast Diffusion Limit

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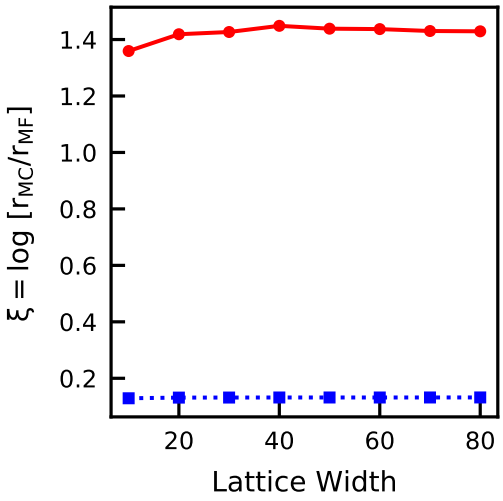

Figure S1: Convergence test of correction term ξ of Monte Carlo ensemble rate vs. the lattice size calculated at $\theta_{CO} = 0.4$, $\theta_O = 0.1$ (red) and $\theta_{CO} = 0.1$, $\theta_O = 0.4$ (blue) on squared lattice.

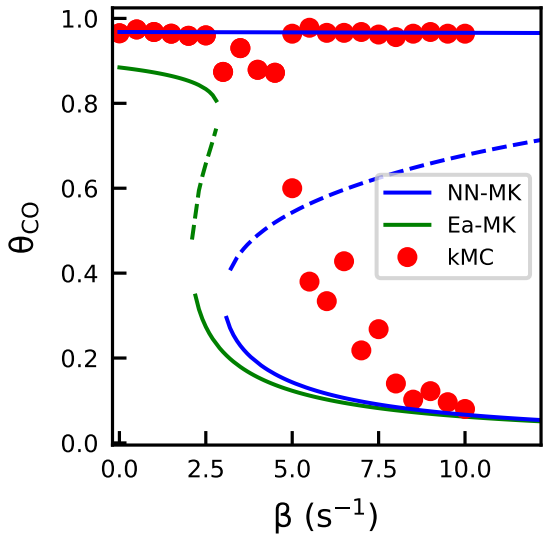

Figure S2: Steady state coverage of coverage of CO* on 1D width=1 when varying oxygen partial pressure (β) predicted by neural network mean field model and kinetic Monte Carlo. Solid line: stable steady state. Dash line: unstable steady state.

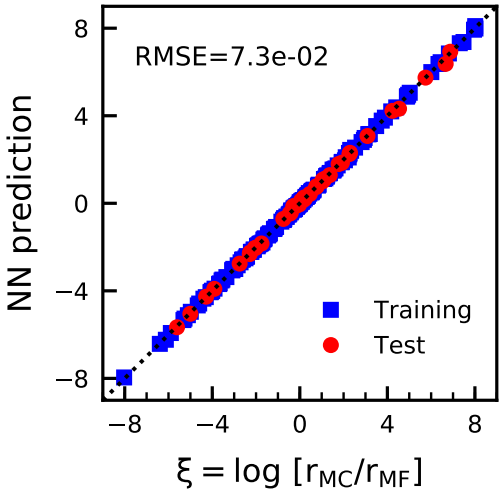

Figure S3: Comparison of the neural network prediction and Monte Carlo simulation of ξ simulated at different coverage values (0 to 1) and different interaction energies (-3 to 3 kcal/mol)