Potential Energy Landscape of CO Adsorbates on NaCl(100) and Implications in Isomerization of Vibrationally Excited CO

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SUPPORTING INFORMATION

Figure S1. Convergence test of DFT parameters. (a) Adsorption potential energies of CO in the *p*(2×2) unit cell calculated with several functionals and different numbers of NaCl(100) slab layers, using a *k*-point mesh of 3×3×1; (b) Adsorption potential energies of CO in the *p*(1×1) unit cell calculated with the PBE-D3(BJ) functional with different values of *k*-point mesh.

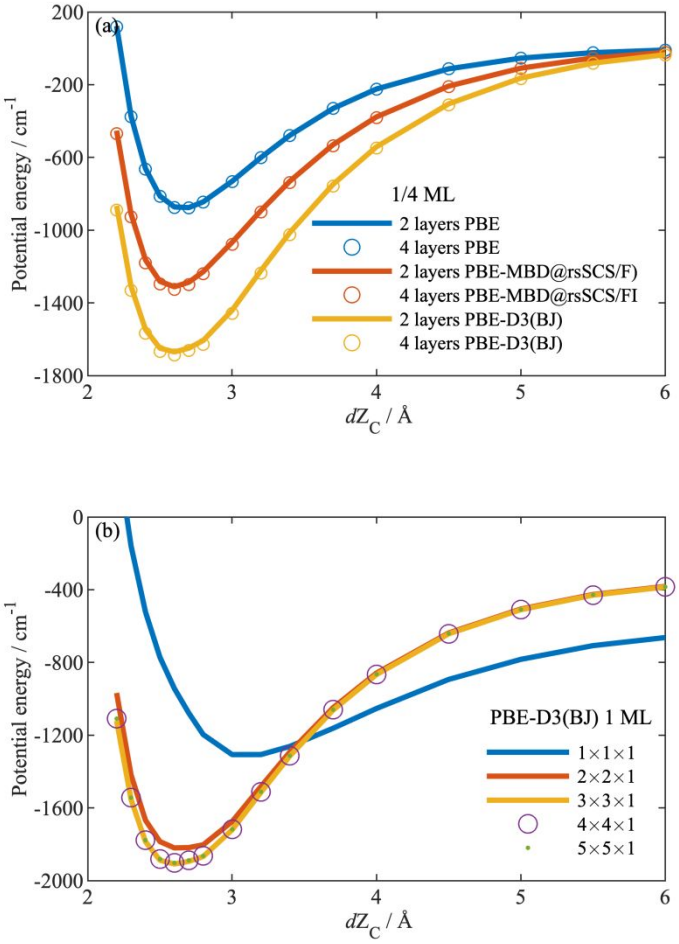

Figure S2. Fitting error distributions of the 2×2-MBD, 2×2-D3, 1×1-MBD and 1×1-D3 PESs.

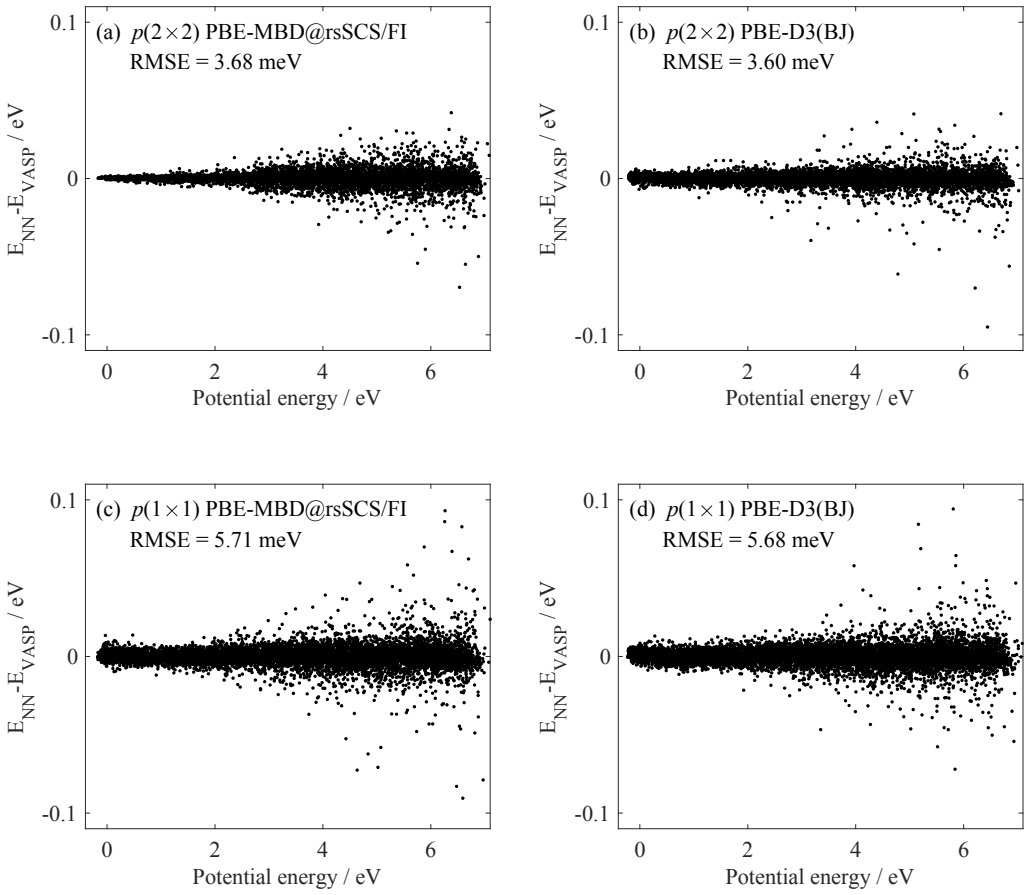

Figure S3. Illustration of configurations “A” to “H” marked in Figures 5 and 7. The Na^+, Cl^-, O and C are represented by blue, yellow, red and gray circles, respectively.