Supplementary information

Direct versus hydrogen-assisted CO dissociation over stepped Ni and Ni₃Fe surfaces: a computational investigation

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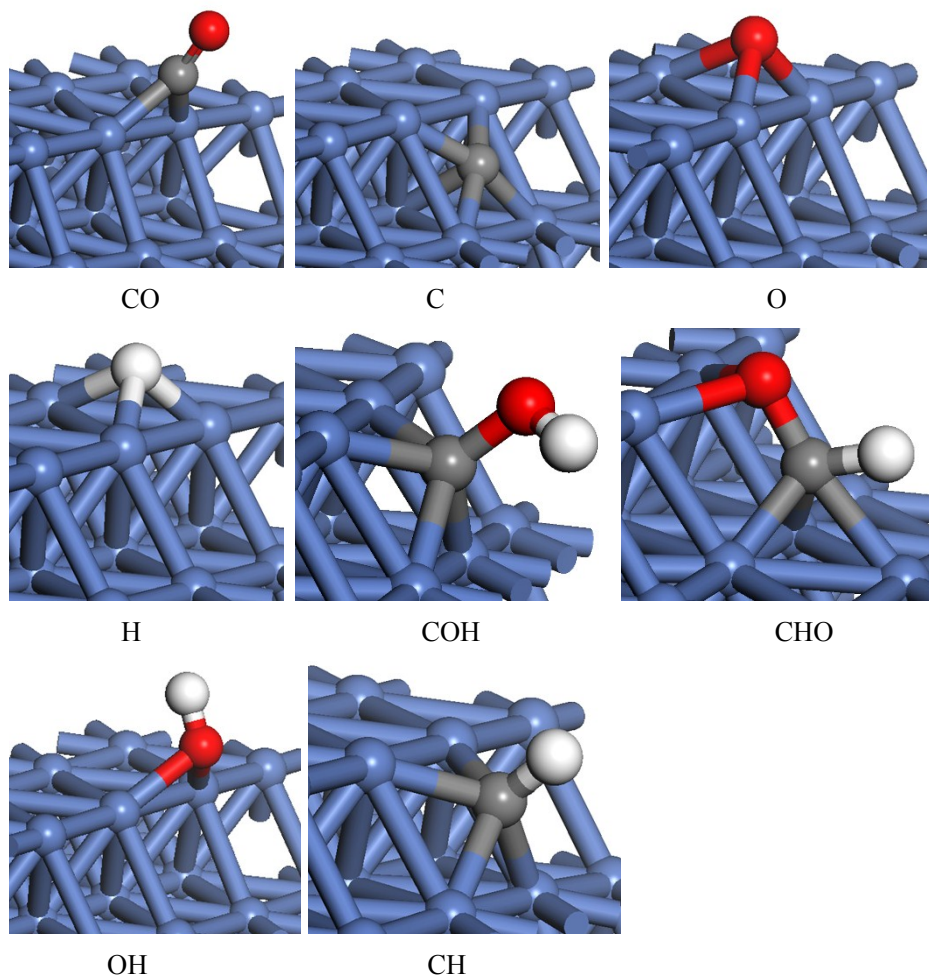E-mail address: yzhyu@tju.edu.cn (Y. Yu)

CO   C   O

H   COH   CHO

OH   CH

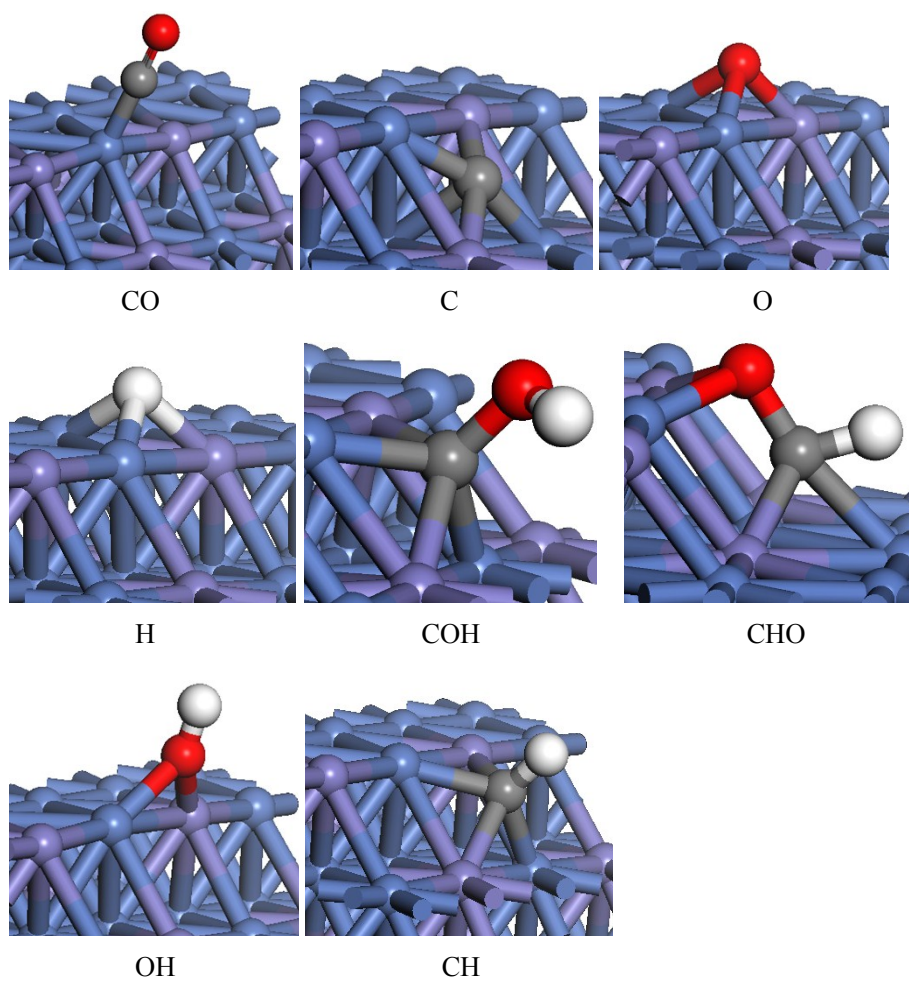Figure S1. Favored adsorption configurations of CO and relevant species on Ni(211)

Figure S2. Favored adsorption configurations of CO and relevant species on Ni$_3$Fe(211)-AB

CO   C   O
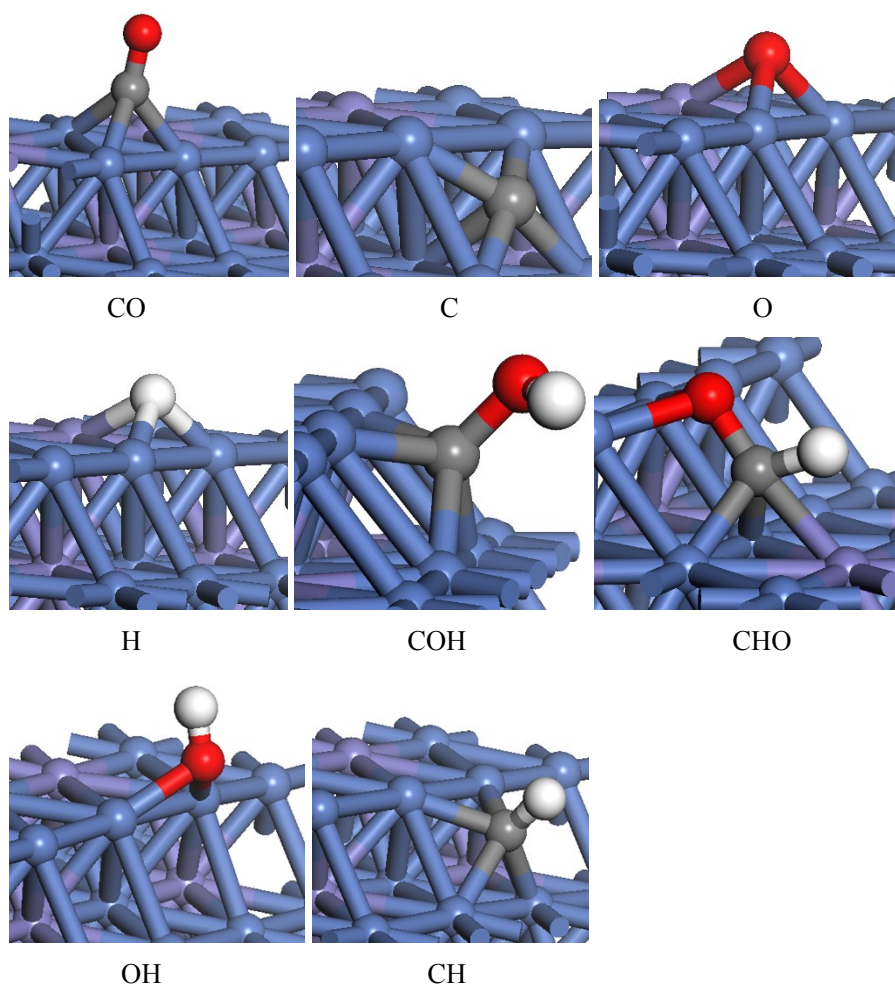
H   COH   CHO

OH   CH

Figure S3. Favored adsorption configurations of CO and relevant species on $Ni_3Fe(211)$-AA

SE-hcp   SE-bridge   4H via C   4H via C and O

0.08 → 0.39 → 0.32 →

← 0.10 ← 0.07 ← 0.22

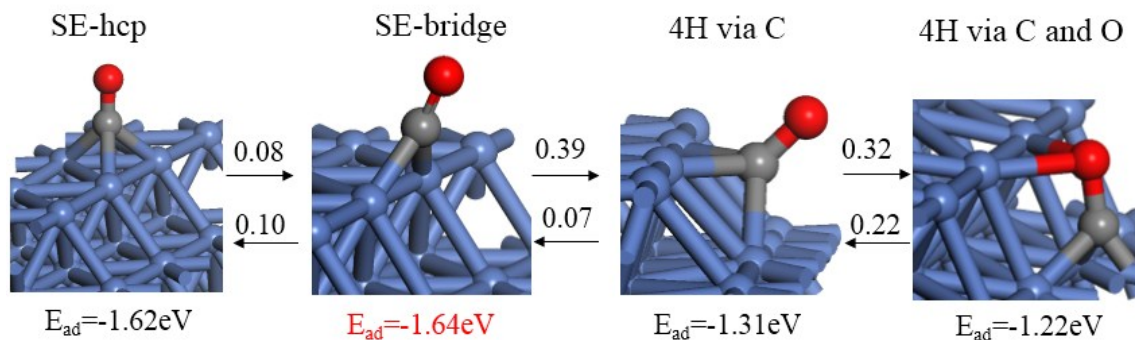$E_{ad}=-1.62eV$ $E_{ad}=-1.64eV$ $E_{ad}=-1.31eV$ $E_{ad}=-1.22eV$

Figure S4. The diffusion of CO between several typical adsorption geometries on Ni(211). The adsorption sites and corresponding adsorption energies are labeled over and below the figures; the diffusion barriers (eV) are marked above the arrows.

SE-bridge   SE-hcp   SE-fcc

0.01 → 0.19 →

← 0.05 ← 0.11

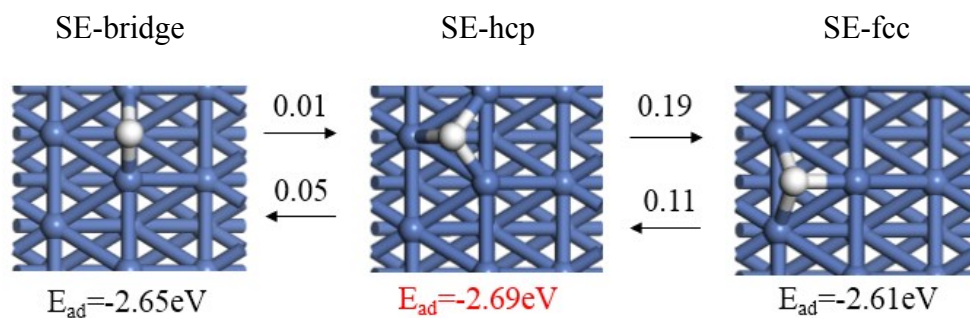$E_{ad}=-2.65eV$ $E_{ad}=-2.69eV$ $E_{ad}=-2.61eV$

Figure S5. The diffusion of H between several typical adsorption geometries on Ni(211). The adsorption sites and corresponding adsorption energies are labeled over and below the figures; the diffusion barriers (eV) are marked above the arrows.