Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information: Oxidation of CO on a Carbon-based Material Composed of Nickel Hydroxide on Hydroxyl Graphene Oxide, ($Ni_4(OH)_3$/hGO) – a First-Principles Calculation

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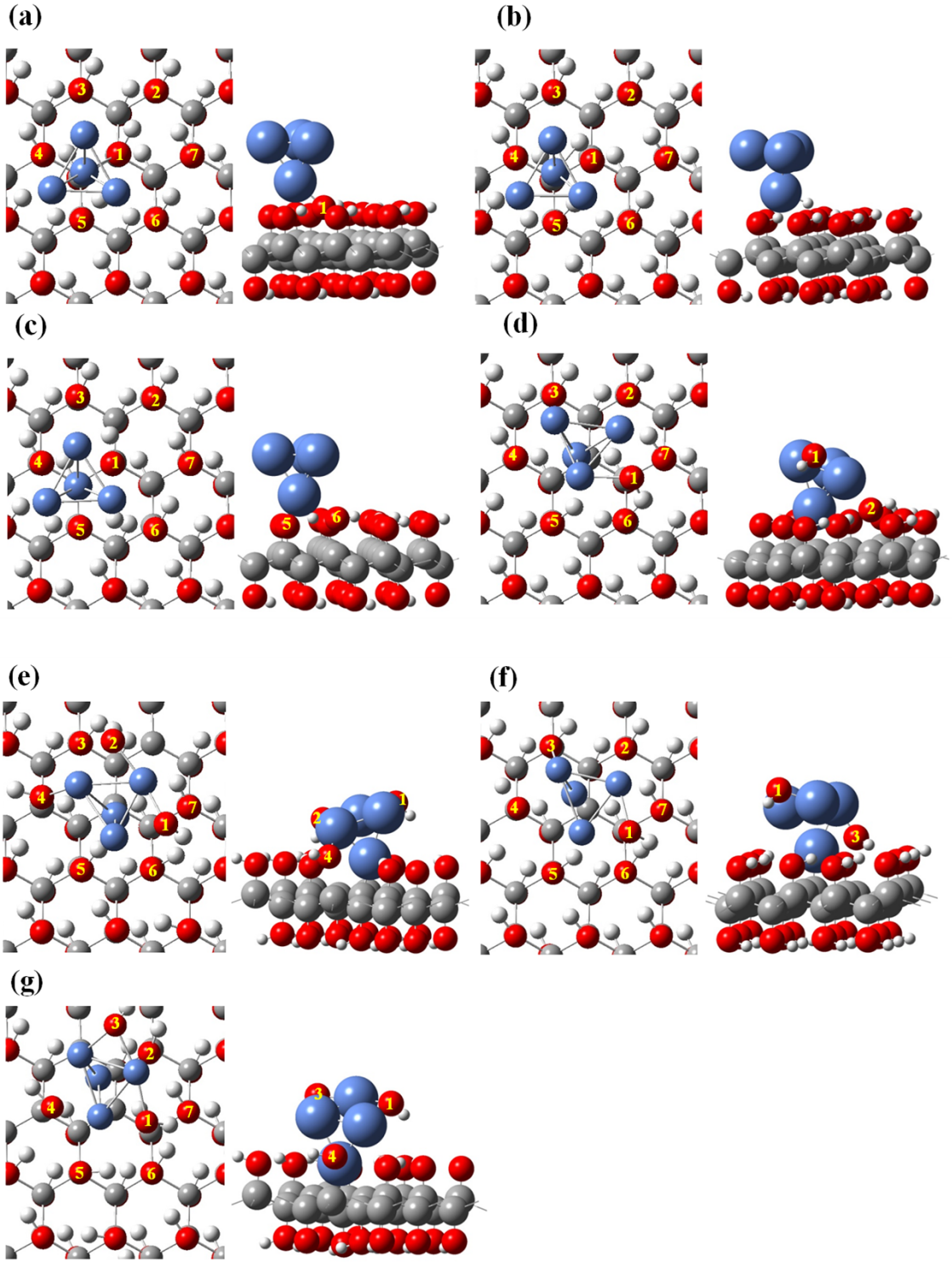

Figure S1. Transition state structures of the reduced mechanism by Ni_4 on hydroxyl graphene oxide (hGO) sheet : (a) $Ni_4OH_{(a)}$ + $hGO_{(s)}$, (b) $Ni_4H_{(a)}$ + $hGO_{(s)}$, (c) $Ni_{4(a)}$ +$H_2O_{(a)}$ + $hGO_{(s)}$, (d) $Ni_4(OH)_{2(a)}$ + $hGO_{(s)}$ (slight distortion), (e) $Ni_4(OH)_{3(a)}$ + $hGO_{(s)}$ (slight distortion), (f) $Ni_4(OH)_{2(a)}$ + $hGO_{(s)}$ (large distortion) and (g) $Ni_4(OH)_{3(a)}$ + $hGO_{(s)}$.

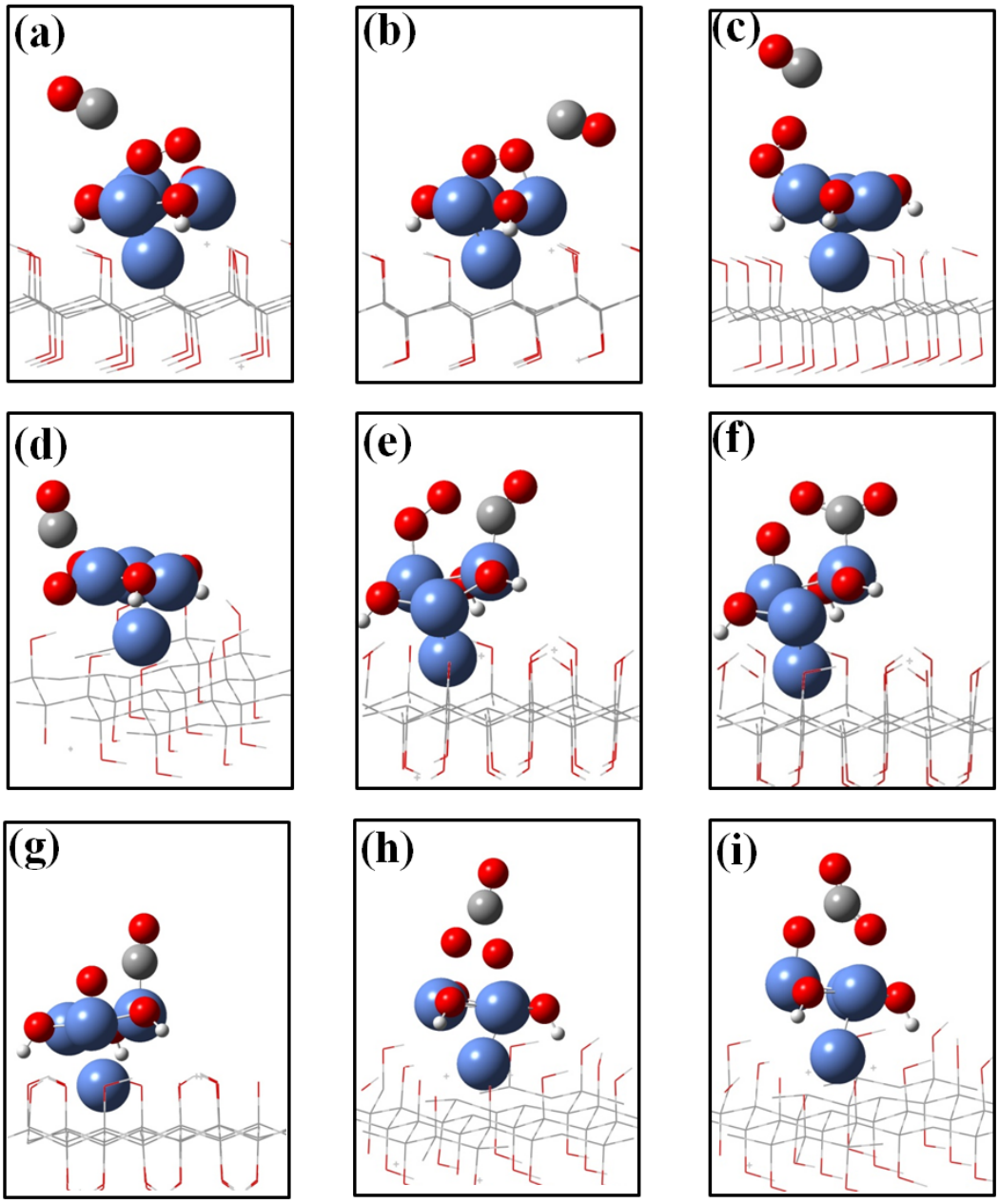

Figure S2. Transition state structures of the CO oxidation reaction on $Ni_4(OH)_3$/hGO sheet : (a) $CO_{(g)} + O_{2(a)}$ [hollow](left) → $CO_{2(g)} + O_{(a)}$, and (b) $CO_{(g)} + O_{2(a)}$ [hollow](right) → $CO_{2(g)} + O_{(a)}$, (c) $CO_{(g)} + O_{2(a)}$ [top] → $CO_{2(g)} + O_{(a)}$, (d) 2^{nd} $CO_{(g)} + O_{(a)}$ [top] → $CO_{2(g)}$, (e) $CO_{(a)} + O_{2(a)}$ → $OCOO_{(a)}$, (f) $OCOO_{(a)}$ → $CO_{2(g)} + O_{(a)}$, (g) 2^{nd} $CO_{(a)} + O_{(a)}$ → $CO_{2(g)}$ (h) $CO_{(g)} + O_{2(a)}$ [hollow] → $CO_{3(g)}$, (i) $CO_{3(g)}$ → $CO_{2(g)} + O_{(a)}$.

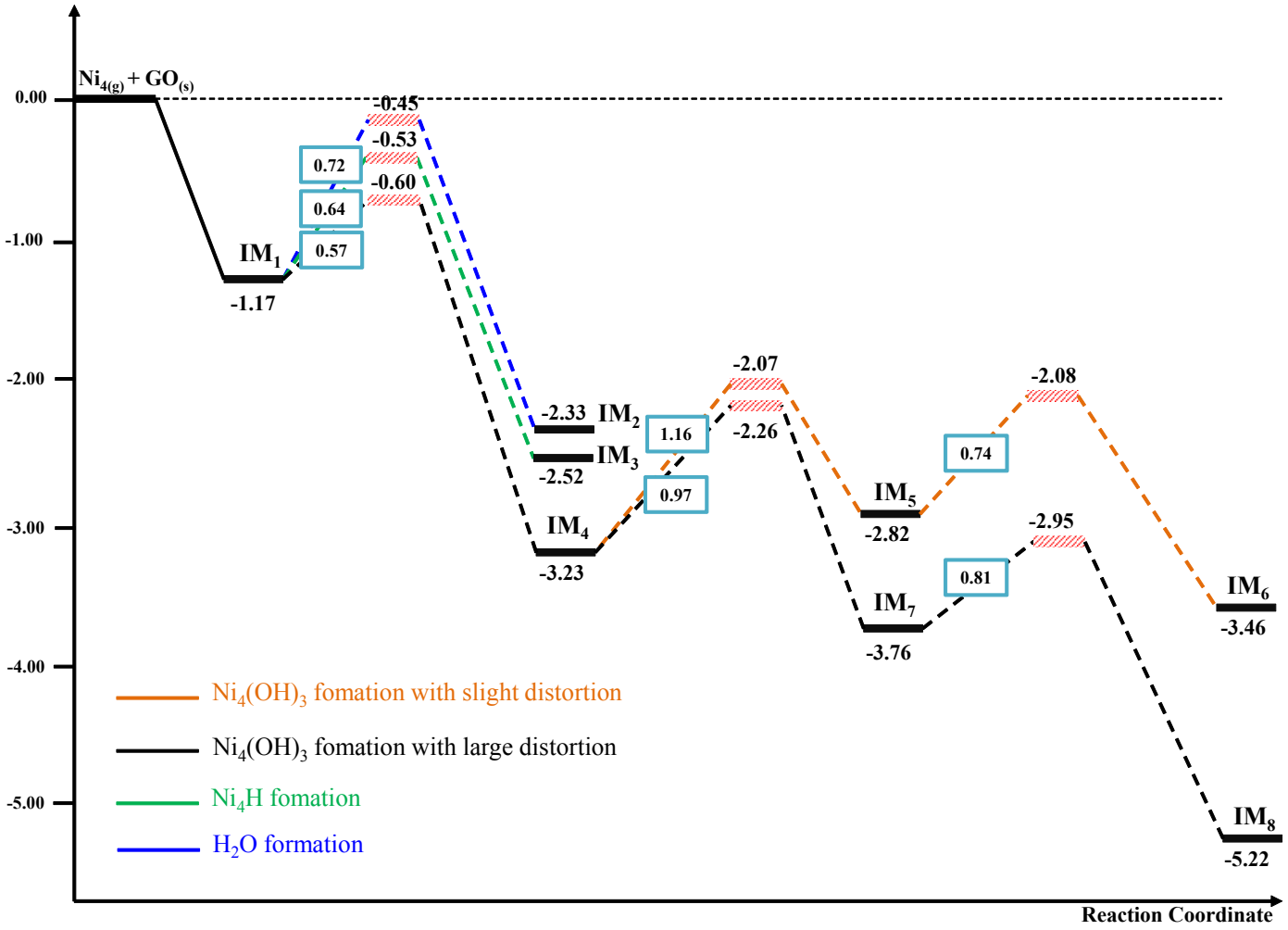

Figure S3. Calculated potential-energy diagram with DFT-D3 correction for the reaction Ni_4/hGO → $Ni_4(OH)_3$/hGO.

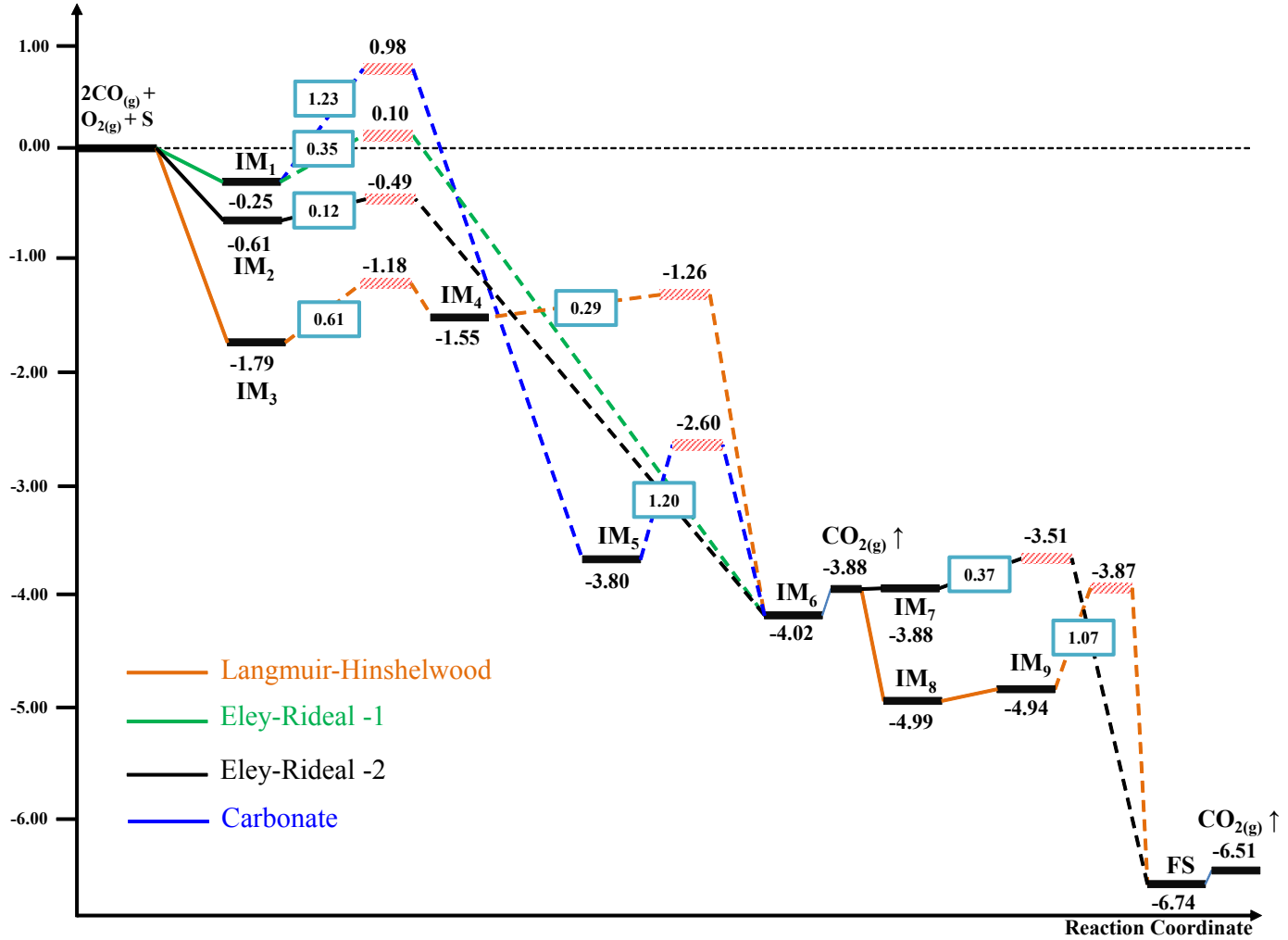

Figure S4. The calculated possible potential energy diagram with DFT-D3 correction for CO oxidation reaction on $Ni_4(OH)_3$/hGO sheet.