Supporting Information

A DFT Study of CO_2 Electroreduction Catalyzed by Hexagonal Boron-Nitride Nanosheets with Vacancy Defects

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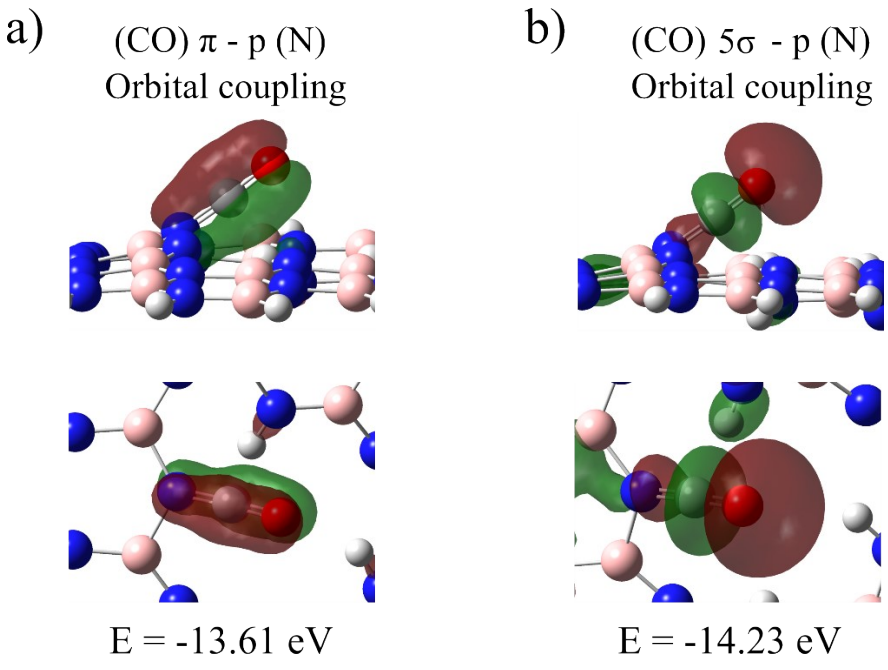

Figure S1. Contour plots of occupied Kohn−Sham orbitals at around -14 eV of V_{B3N}-CO adduct. Green and maroon areas indicate the change of the sign of the orbitals.

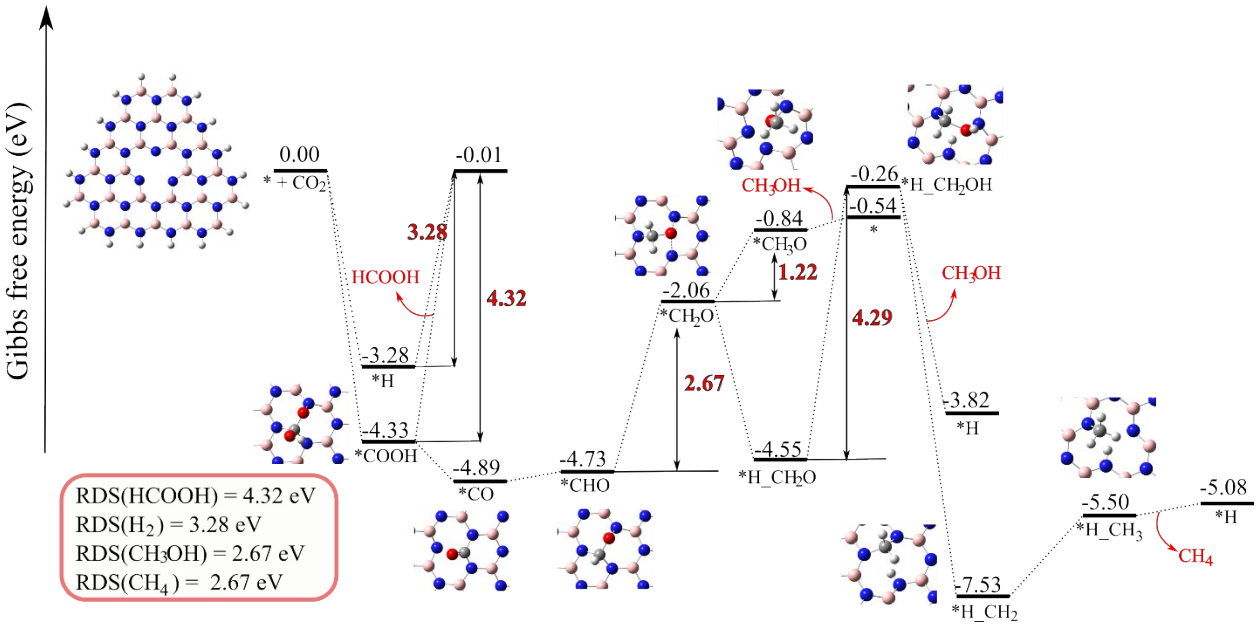

Figure S2. The free-energy changes (ΔG_{sol}) were calculated for the electrochemical pathways, for the reduction of CO_2, on the V_B monovacancy of *h*-BN using the CHE model. There are ten ($H^+ + e^-$) pair transfers to CO_2.

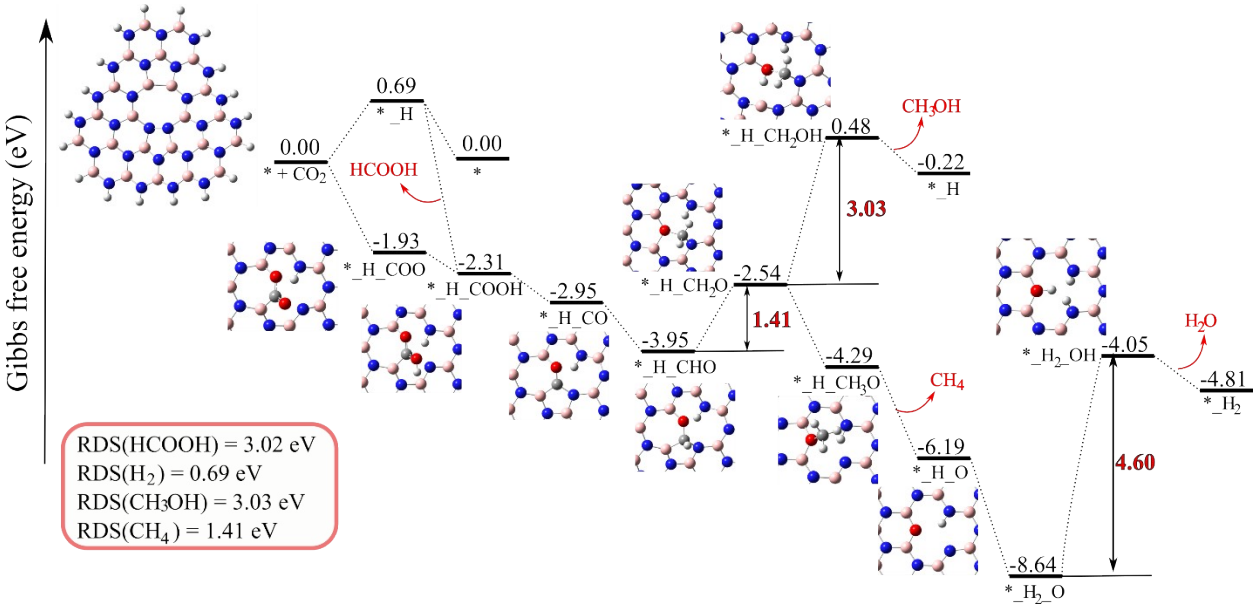

Figure S3. The free-energy changes (ΔG_{sol}) were calculated for the electrochemical pathways, for the reduction of CO_2, on the V_{BN} divacancy of *h*-BN using the CHE model. There are ten ($H^+ + e^-$) pair transfers to CO_2.

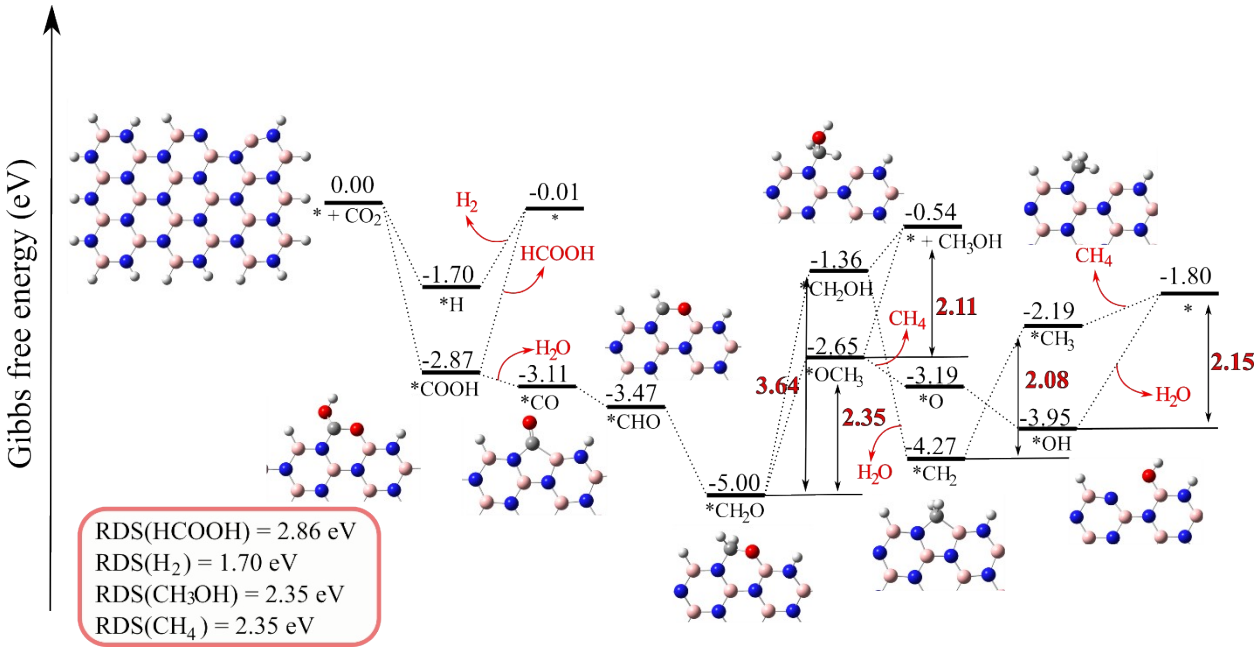

Figure S4. The free-energy changes (ΔG_{sol}) were calculated for the electrochemical pathways, for the reduction of CO_2, on the *armchair* conformation of *h*-BN nanosheet edges using the CHE model. There are eight ($H^+ + e^-$) pair transfers to CO_2.