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

Supporting information for: Single B-Vacancy Enriched α_1-Borophene Sheet: An Efficient Metal-Free Electrocatalyst for CO_2 Reduction

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Table S1: Values of zero-point energy (ZPE) and TS at T = 298.15 K for different adsorbed intermediates for C_1-redution of CO_2 over the α_{1-t1}-borophene surface in the units of eV.

	Gas Phase		Solvent Phase	
Species	ZPE	TS	ZPE	TS
$*CO_2$	0.34	0.13	0.34	0.13
*COOH	0.67	0.14	0.67	0.15
HCOO*	0.67	0.13	0.67	0.13
*CO	0.22	0.15	0.22	0.15
H_2COO*	0.98	0.13	0.98	0.13
*CHO	0.48	0.17	0.49	0.16
$H_2C(OH)O*$	1.28	0.15	1.29	0.15
$*CH_2O$	0.89	0.08	0.84	0.08
$*CH_2OH$	1.11	0.18	1.11	0.18
$*OCH_3$	1.11	0.15	1.11	0.14
$*CH_2$	0.67	0.08	0.67	0.09
$*CH_3$	0.98	0.12	0.97	0.12
$*O + *CH_4$	1.30	0.26	1.31	0.25
*OH	0.38	0.07	0.38	0.07

Table S2: Values of zero-point energy (ZPE) and TS at T = 298.15 K for different adsorbed intermediates for C_2-redution of CO_2 over the α_{1-t1}-borophene surface in the units of eV.

	Gas Phase		Solvent Phase	
Species	ZPE	TS	ZPE	TS
*CO + *CO	0.45	0.28	0.45	0.28
*[C(O)- - -CO]	0.40	0.24	0.41	0.22
*[C(O)CO]	0.45	0.22	0.46	0.20
*[C(OH)CO]	0.77	0.20	0.77	0.20
*[CCO]	0.34	0.21	0.34	0.20
*[CHCO]	0.61	0.17	0.61	0.17
*[CHCOH]	0.96	0.15	0.96	0.15
*[CHCHO]	0.98	0.13	0.98	0.13
*[CHCHOH]	1.27	0.13	1.27	0.17
*[CH_2CHO]	1.25	0.18	1.24	0.12
*[CH_2CHOH]	1.55	0.25	1.55	0.16
*[CH_3CHO]	1.52	0.25	1.51	0.23
*[CH_2CH_2OH]	1.87	0.26	1.87	0.27
*[CH_3CH_2O]	1.87	0.27	1.87	0.27
*[CHC]	0.53	0.08	0.53	0.08
*[CHCH]	0.85	0.08	0.85	0.08
*[CH_2CH]	1.17	0.06	1.17	0.06
*[CH_2CH_2]	1.47	0.11	1.47	0.12
*[CH_3CH_2]	1.74	0.20	1.74	0.20

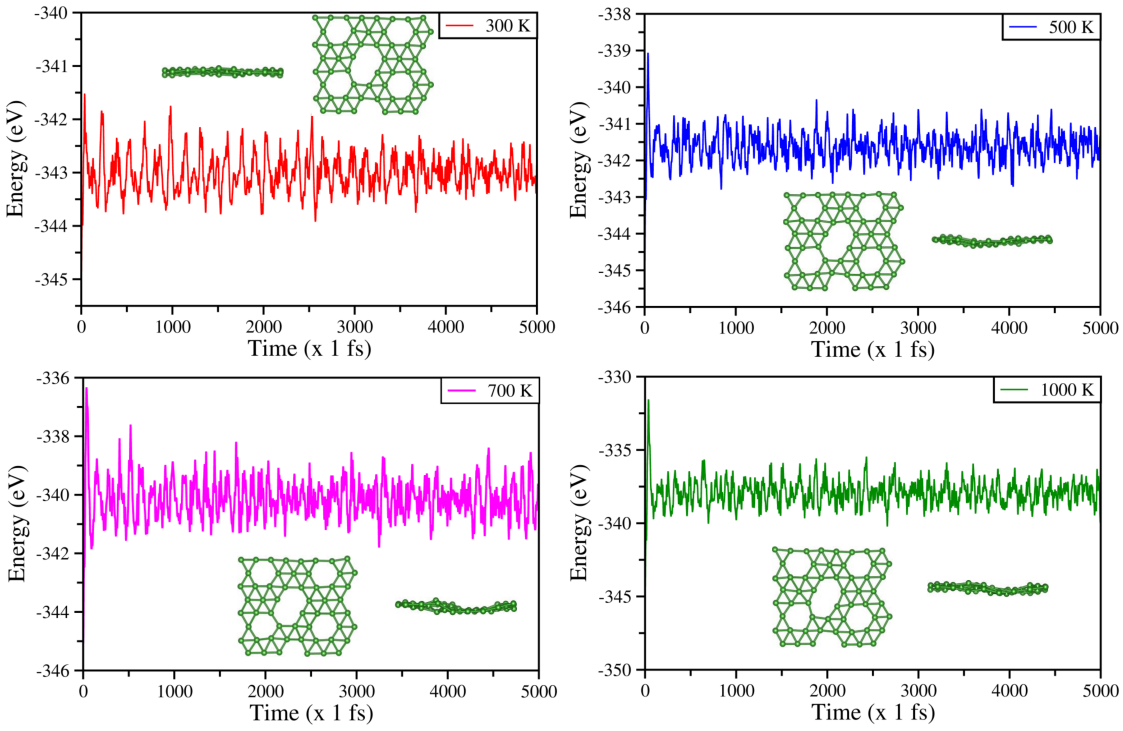

Figure S1: Energy variation plots with time for AIMD simulations of α_{1-t1}-borophene run at 300 K, 500 K, 700 K and 1000 K for 5 ps with a timestep of 1 fs. In the insets of each plot, top and side views of final configurations of α_{1-t1}-borophene sheet after 5 ps are shown.

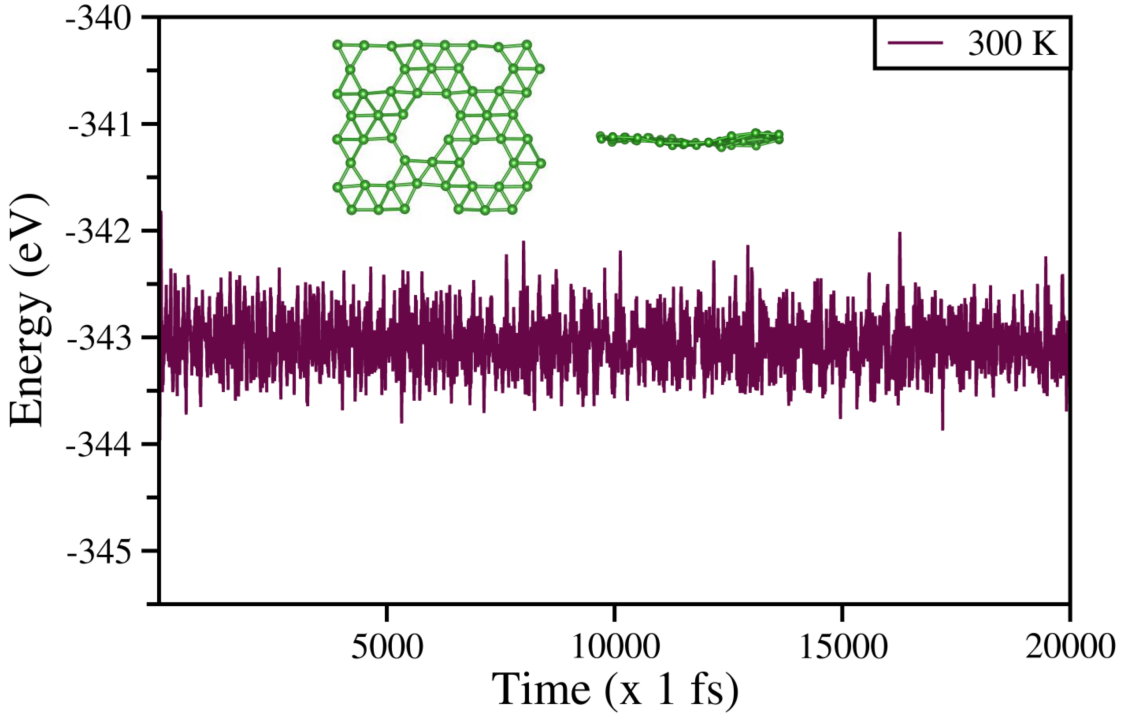

Figure S2: Energy variation plot with time for AIMD simulation of α_{1-t1}-borophene run at 300 K for 20 ps with a timestep of 1 fs. In the inset of the plot, top and side views of final configurations of α_{1-t1}-borophene sheet after 20 ps are shown.

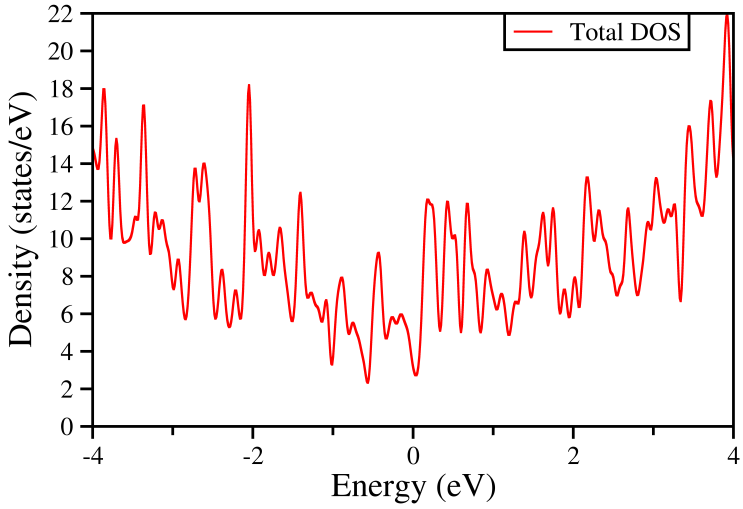

Figure S3: Electronic total density of states plot of α_{1-t1}-borophene calculated from HSE06 level of theory (the Fermi level is shifted to zero).

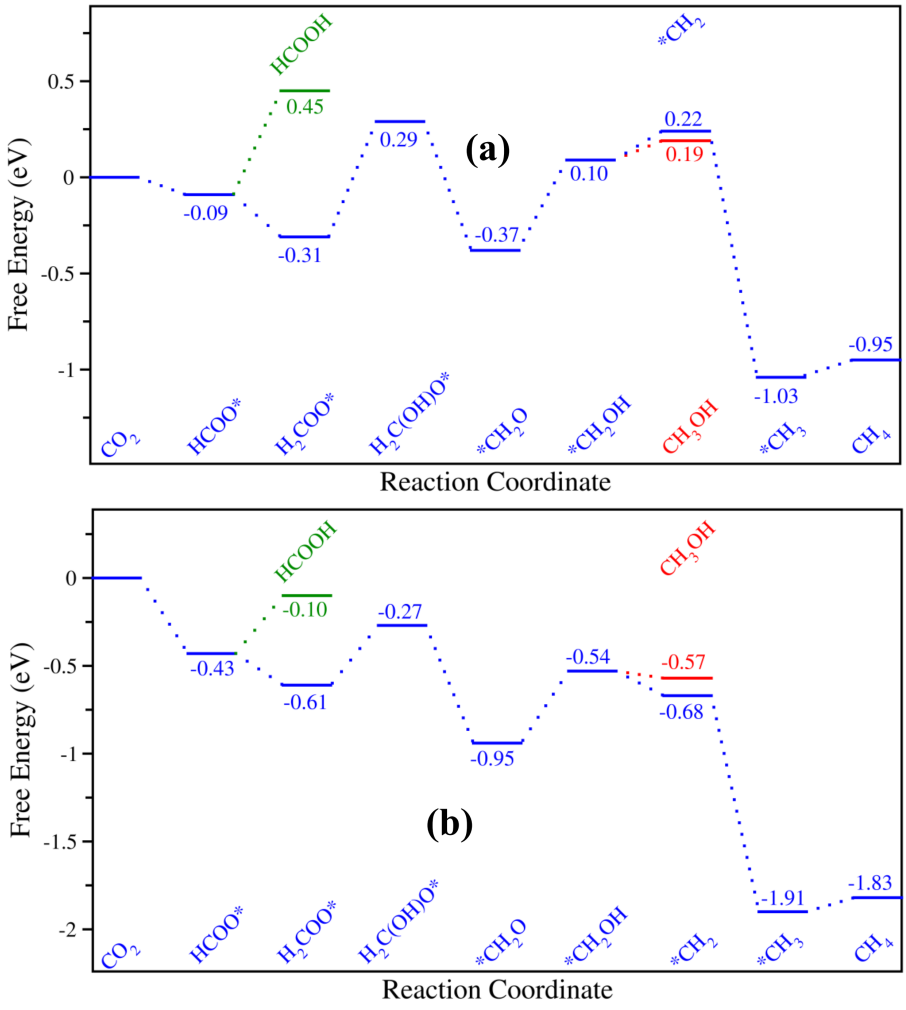

Figure S4: Relative free energy diagram for conversion of CO_2 into C_1-products (HCOOH, CH_3OH and CH_4) via formation of HCOO intermediate over the α_{1-t1}-borophene surface, calculated in (a) gas phase and (b) solvent phase.

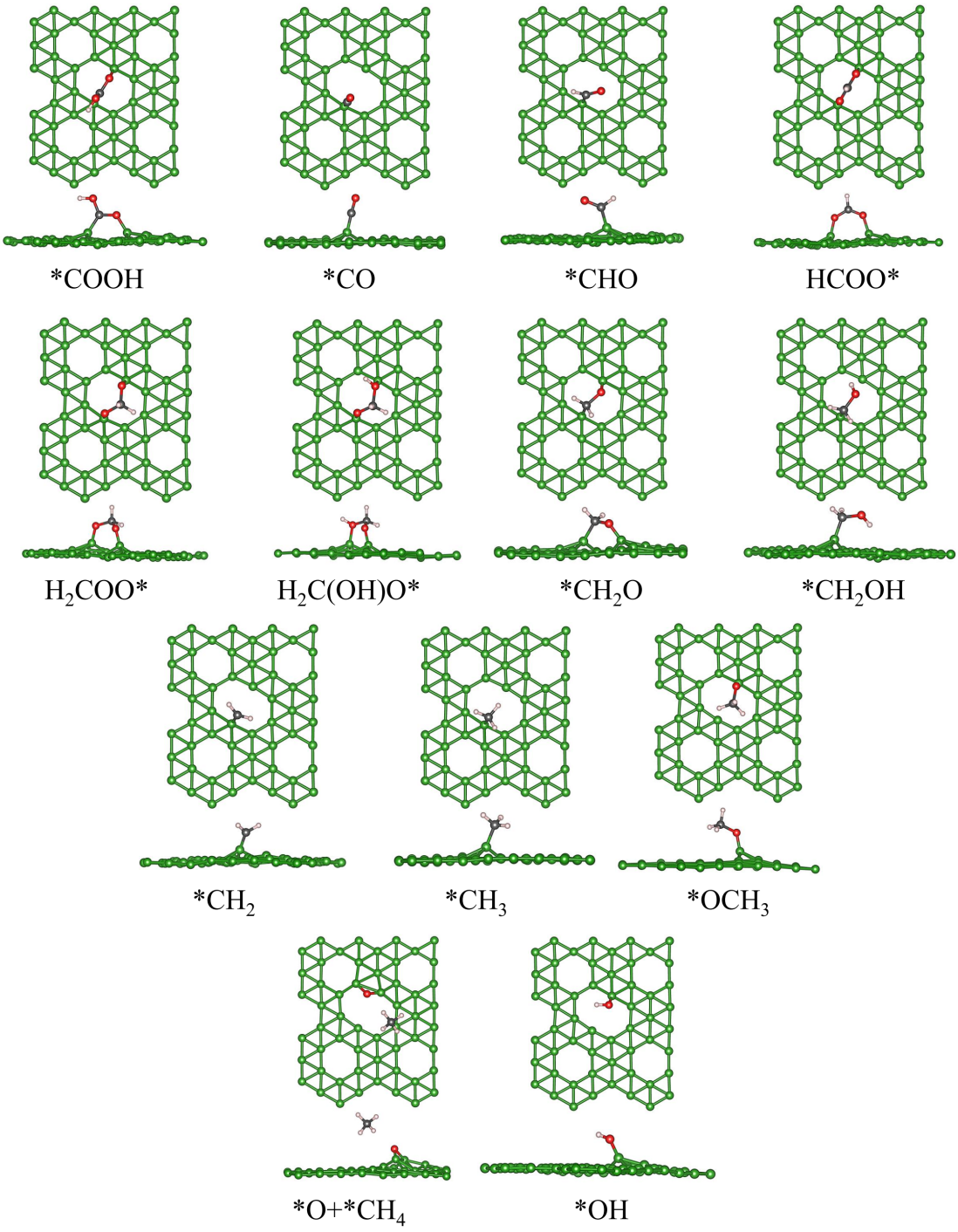

Figure S5: Electronic structures of intermediates for conversion of adsorbed CO_2 leading to C_1-products. The green, grey, red and white balls represent B, C, O and H atoms respectively.

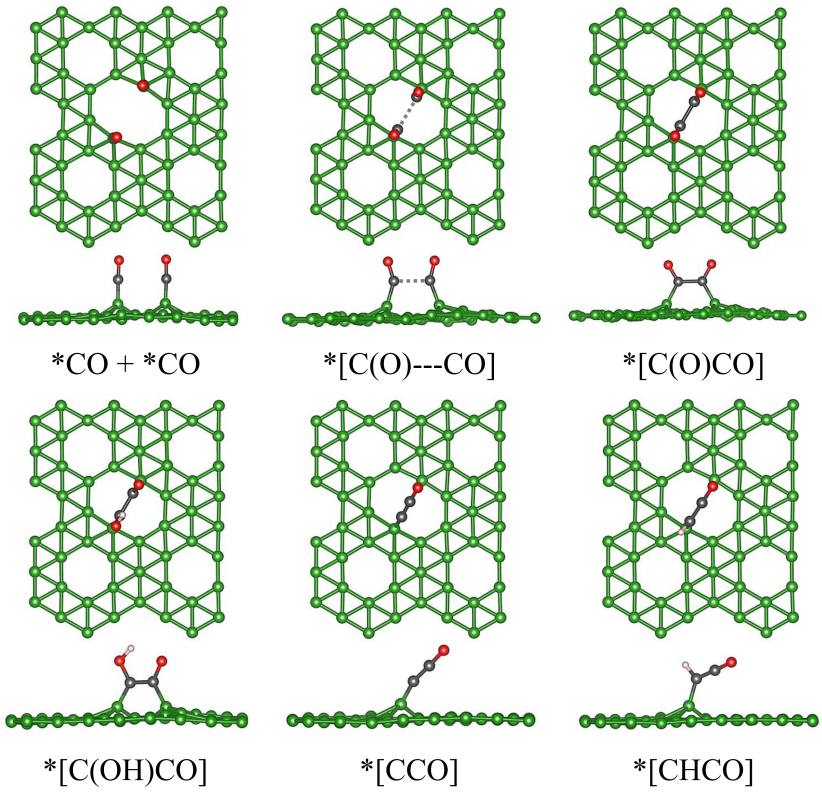

Figure S6: Optimized geometries of transition state and intermediates for coupling of two adsorbed CO followed by further conversion into adsorbed CHCO intermediate. The green, grey, red and white balls represent B, C, O and H atoms respectively.

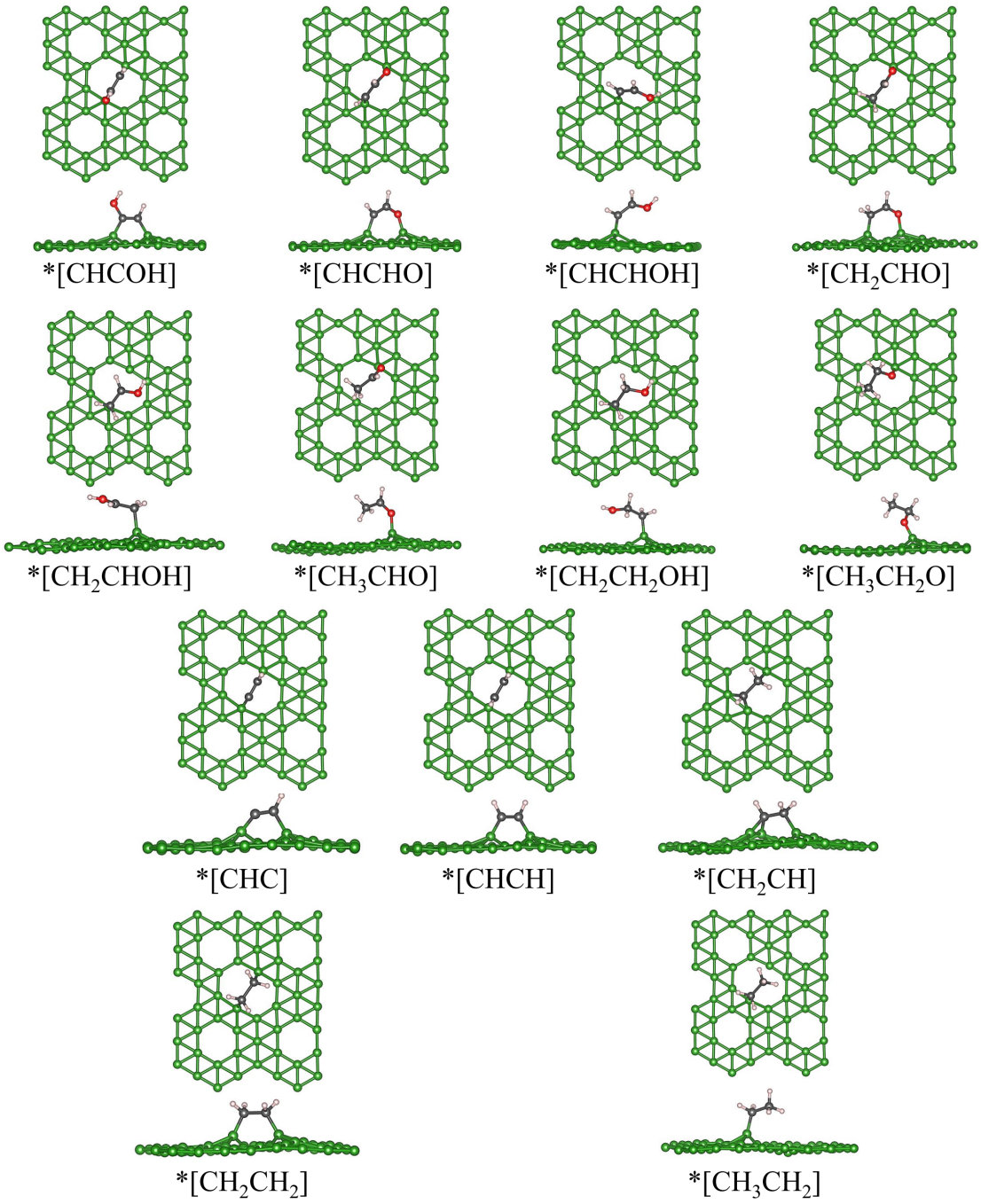

Figure S7: Optimized geometries of intermediates for the hydrogenations of *[CHCO] leading to C_2-products. The green, grey, red and white balls represent B, C, O and H atoms, respectively.