Electronic Supplementary Material (ESI) for Materials Advances.

Computational Insights into Selective CO_2 Hydrogenation to CH_3OH Catalysed by ZnO Based Nanocages

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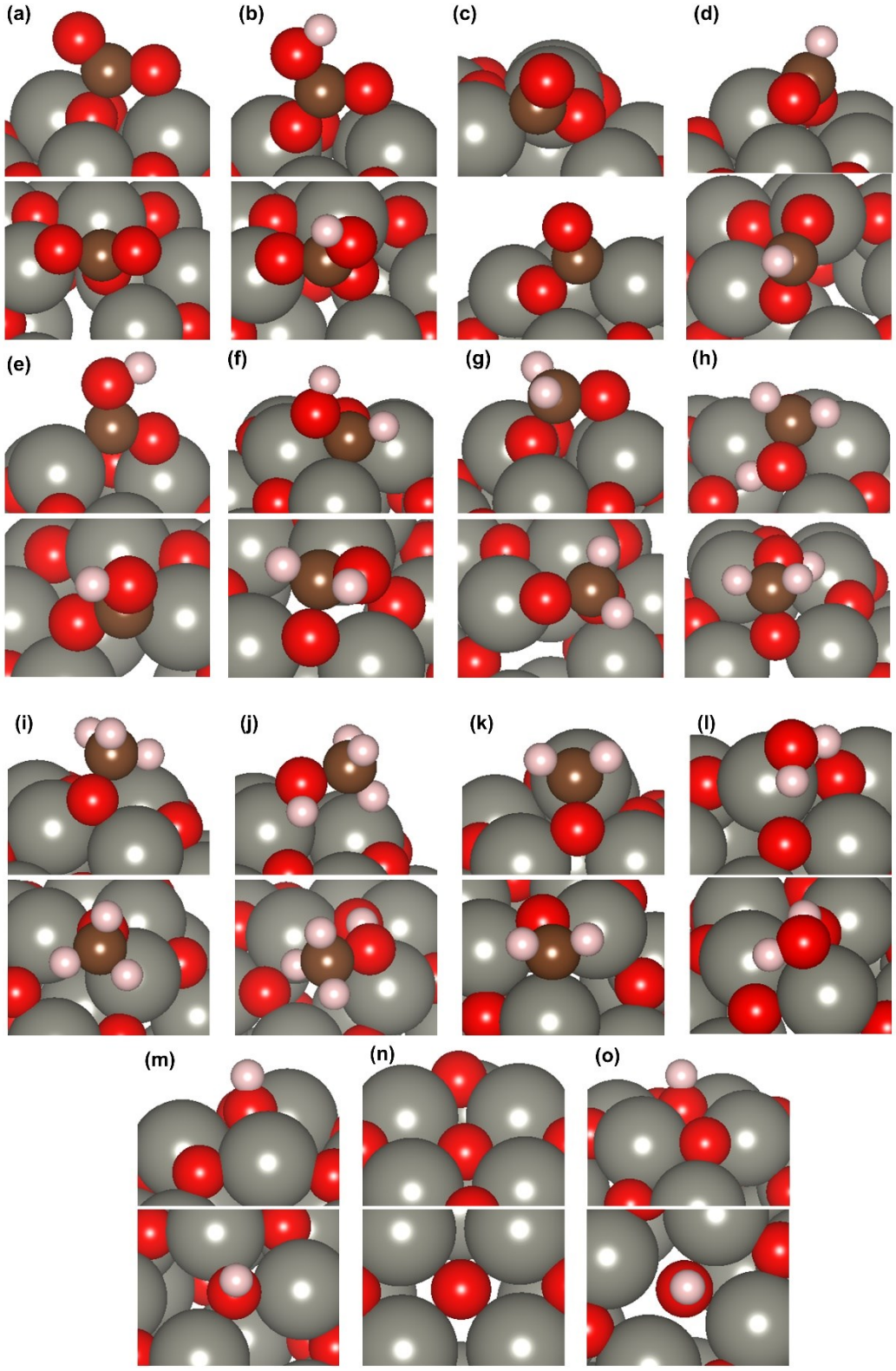

Figure S1: Adsorption patterns of the considered CO_2 hydrogenation reaction intermediates on ZnO NC: (a) *CO_2, (b) *COOH, (c) *CO, (d) *CHO, (e) *COH, (f) *CHOH, (g) *CH_2O, (h) *CH_2OH, (i) *CH_3O, (j) *CH_3OH, (k) *CH_2, (l) *H_2O, (m) *H, (n) *O and (o) *OH.

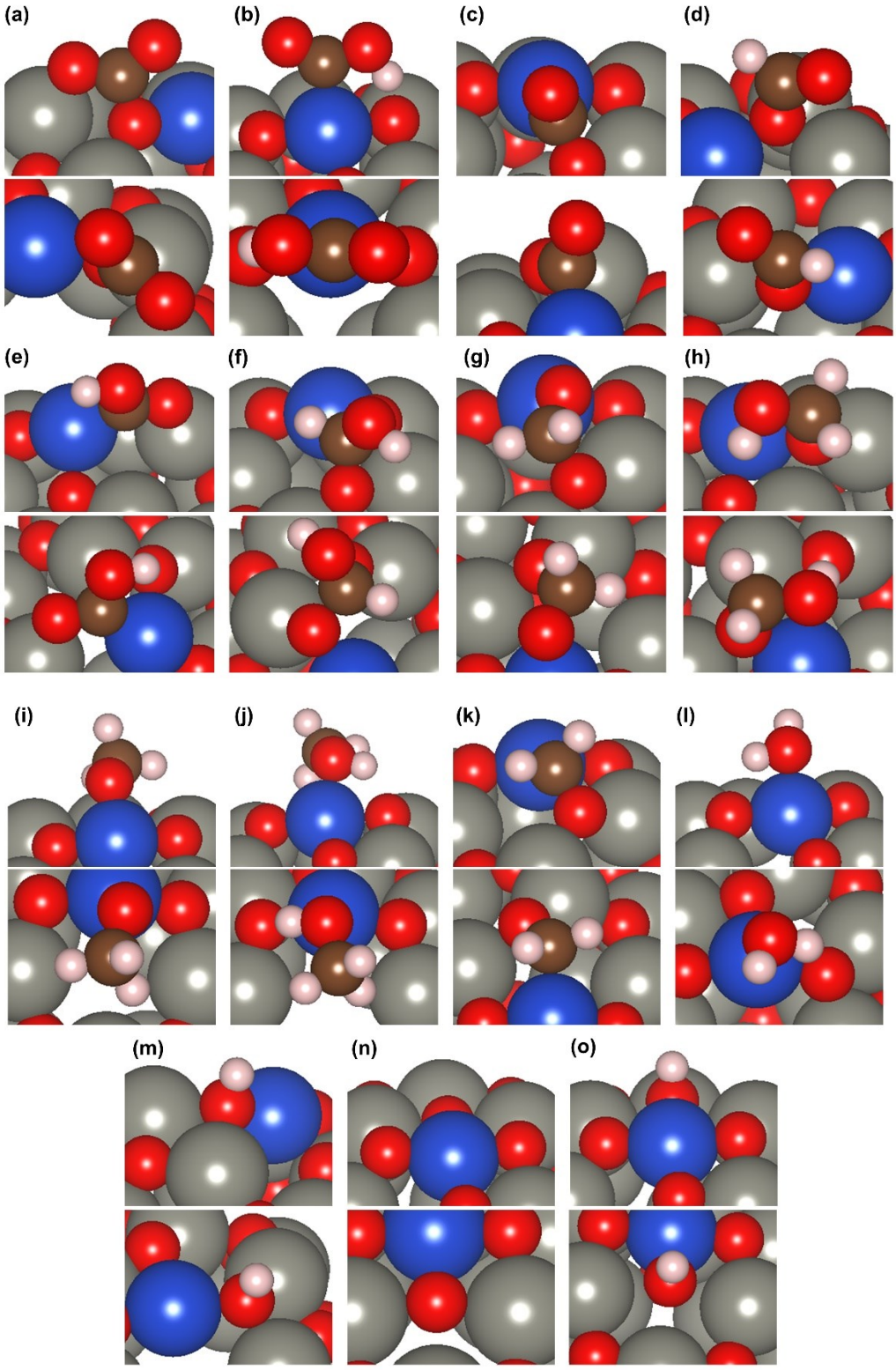

Figure S2: Adsorption patterns of the considered CO_2 hydrogenation reaction intermediates on Cu@ZnO NC: (a) *CO_2, (b) *COOH, (c) *CO, (d) *CHO, (e) *COH, (f) *CHOH, (g) *CH_2O, (h) *CH_2OH, (i) *CH_3O, (j) *CH_3OH, (k) *CH_2, (l) *H_2O, (m) *H, (n) *O and (o) *OH.

Table S1: Calculated electronic energy, ZPE correction and ZPE corrected reaction energy of considered intermediates for CO_2 hydrogenation reaction to CH_3OH by ZnO NC. All energies are in eV.

Intermediates	Energy	ZPE corrections	ZPE corrected reaction energy
ZnO NC	-198.8320	-	-198.8320
CO_2	-22.9622	0.3062	-22.6560
H_2	-6.7686	0.2679	-6.5007
H	-3.3843	0.1339	-3.2504
*CO_2	-222.0834	0.2296	-221.8538
*COOH	-225.4550	0.5755	-224.8795
*CO	-214.0428	0.1087	-213.9341
H_2O	-14.2188	0.5684	-13.6504
*CHO	-217.9717	0.3625	-217.6092
*COH	-217.1852	0.3756	-216.8096
*CH_2O	-221.8826	0.6717	-221.2109
*CHOH	-221.0812	0.6997	-220.3815
*CH_3O	-224.2807	1.0103	-223.2704
*CH_2OH	-225.2234	1.0312	-224.1922
*CH_2	-214.2784	0.4617	-213.8197
*CH_3OH	-229.7218	1.3697	-228.3521
O_2	-9.8454	-	-9.8454
O	-4.9227	-	-4.9227
CH_3OH	-30.2253	1.3567	-28.8686

Table S2: Calculated electronic energy, ZPE correction and ZPE corrected reaction energy of considered intermediates for CO_2 hydrogenation reaction to CH_3OH by Cu@ZnO NC. All energies are in eV.

Intermediates	Energy	ZPE corrections	ZPE corrected reaction energy
Cu@ZnO NC	-199.6432	-	-199.6432
CO_2	-22.9622	0.3062	-22.6560
H_2	-6.7686	0.2679	-6.5007
H	-3.3843	0.1339	-3.2504
*CO_2	-222.9462	0.2269	-222.7193
*COOH	-226.0777	0.4953	-225.5824
*CO	-215.3012	0.1090	-215.1922
H_2O	-14.2188	0.5684	-13.6504
*CHO	-219.2358	0.3680	-218.8678
*COH	-219.0440	0.3810	-218.6630
*CH_2O	-222.6953	0.6636	-222.0317
*CHOH	-222.4853	0.7126	-221.7727
*CH_3O	225.7869	0.9964	-224.7905
*CH_2OH	-226.5876	1.0233	-225.5643
*CH_2	-215.5456	0.4641	-215.0815
*CH_3OH	-230.4229	1.3615	229.0614
O_2	-9.8454	-	-9.8454
O	-4.9227	-	-4.9227
CH_3OH	-30.2253	1.3567	-28.8686