Supporting Information

Visible/Infrared Light-Driven High-efficiency CO_2 conversion into Ethane based on B-Co Synergistic Catalyst

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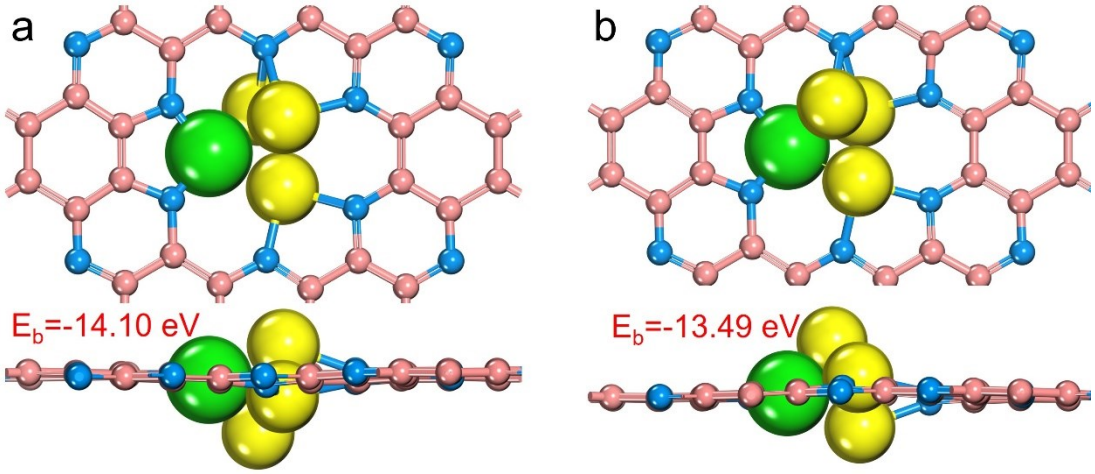

Figure S1. Two possible $BCo_3@C_2N$ configurations, where the green and yellow present B and Co atoms, respectively.

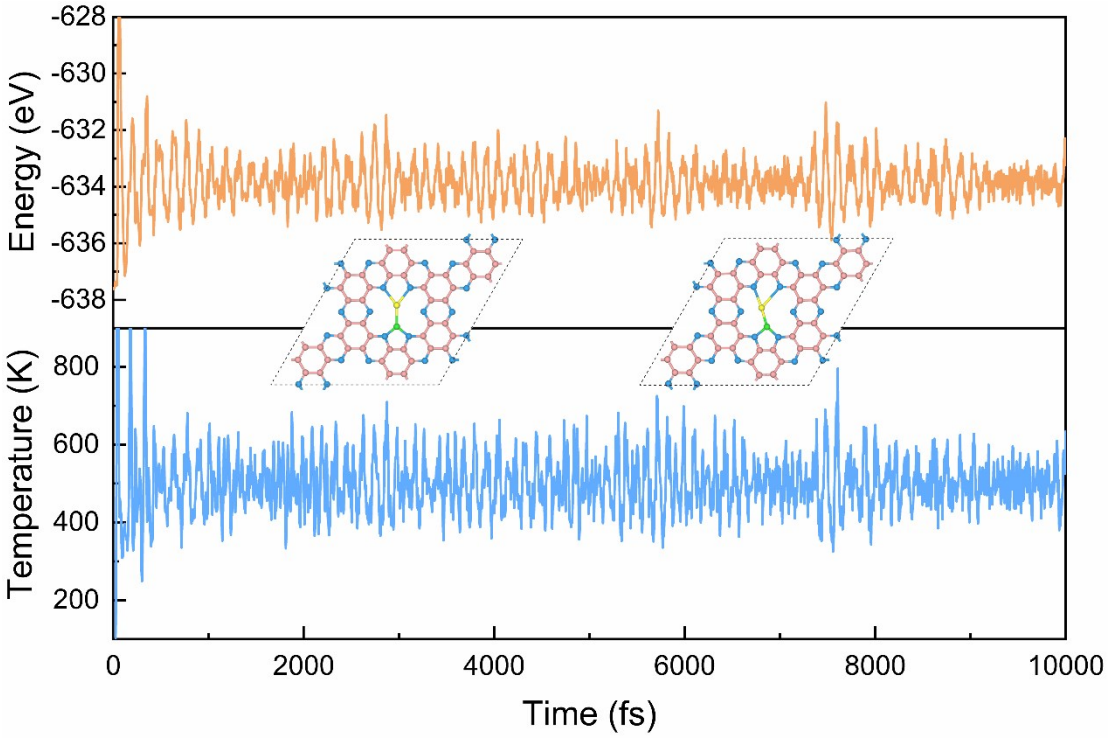

Figure S2. Fluctuation of temperature and energy with respected to the time for AIMD simulations of B-Co@C_2N under 500 K temperature and 2fs time step. The snapshots at the beginning and the end of the trajectory are also shown. The C, N, B, and Co atoms were presented in pink, blue, green and yellow, respectively.

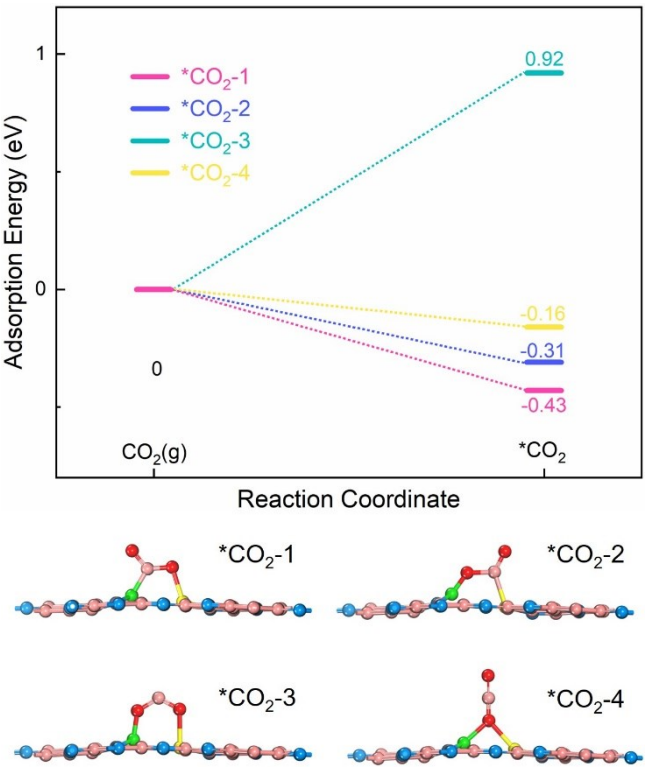

Figure S3. CO_2 adsorption energies of four possible initial CO_2 adsorption configurations on B-Co@C_2N.

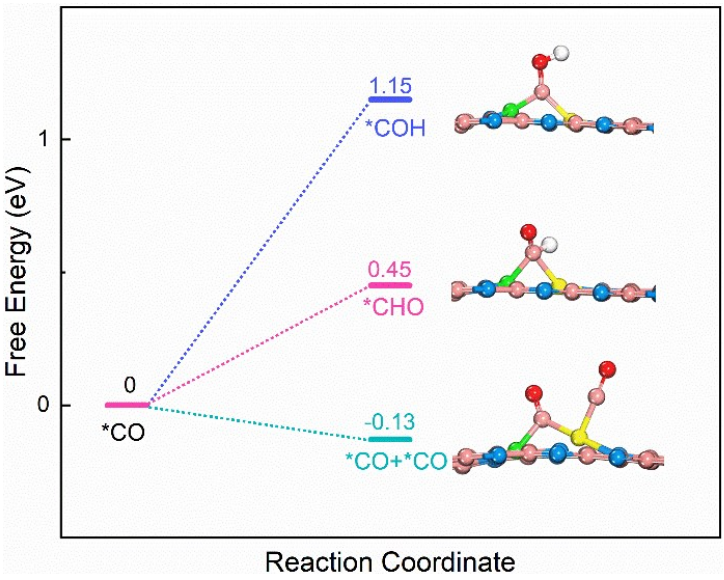

Figure S4. The free energy changes for the further reaction of adsorbed CO molecule.

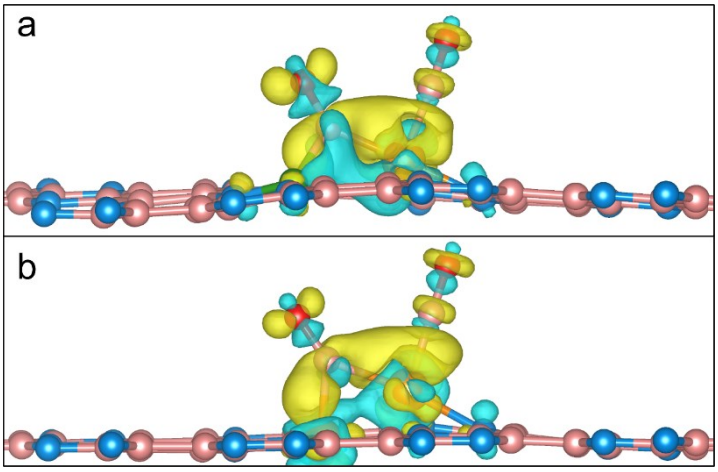

Figure S5. The charge density differences of adsorbed two CO molecules on (a) B-Co@C_2N and (b) Co-Co@C_2N, where the isosurface level is set to 0.005 e/Å^3. Yellow and blue isosurfaces are represented as electron donation and accumulation, respectively.

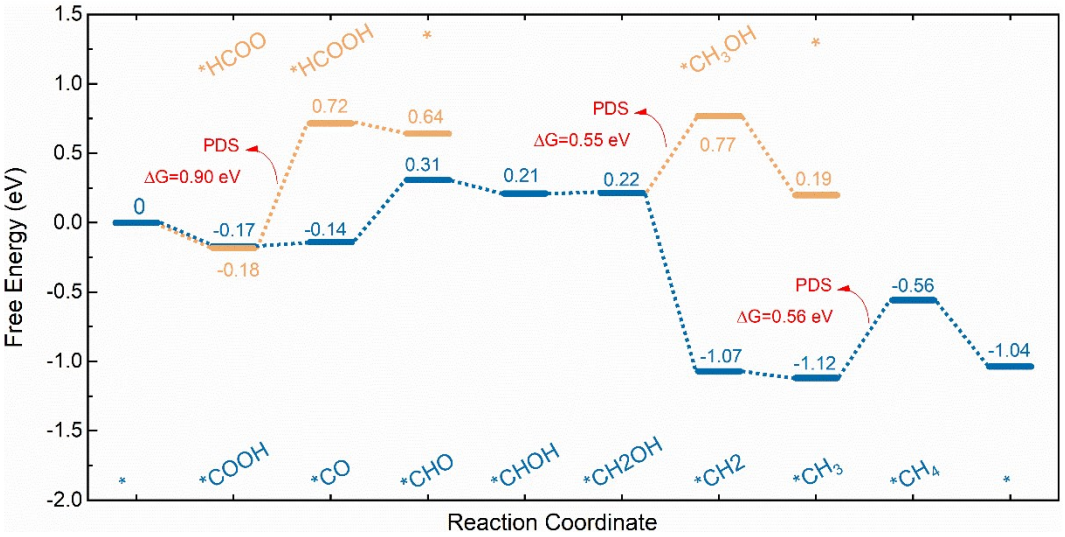

Figure S6. Free energy profiles for CO_2RR toward C_1 products along various possible routes.

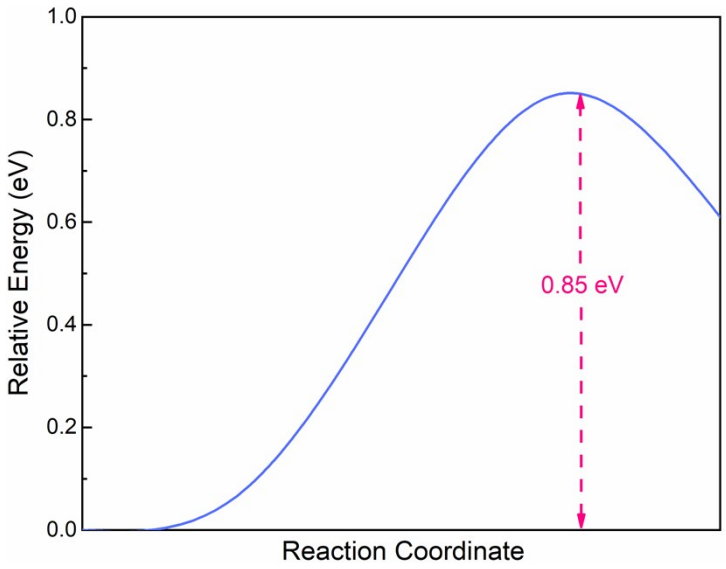

Figure S7. The calculated C-C coupling reaction barrier on B-Co@C_2N through CINEB method.

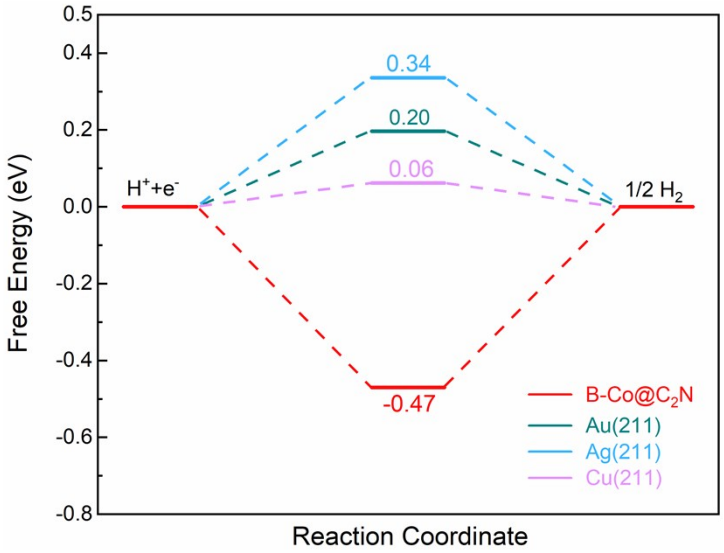

Figure S8. The calculated HER free energy of B-Co@C_2N, Au (211), Ag (211), and Cu (211).

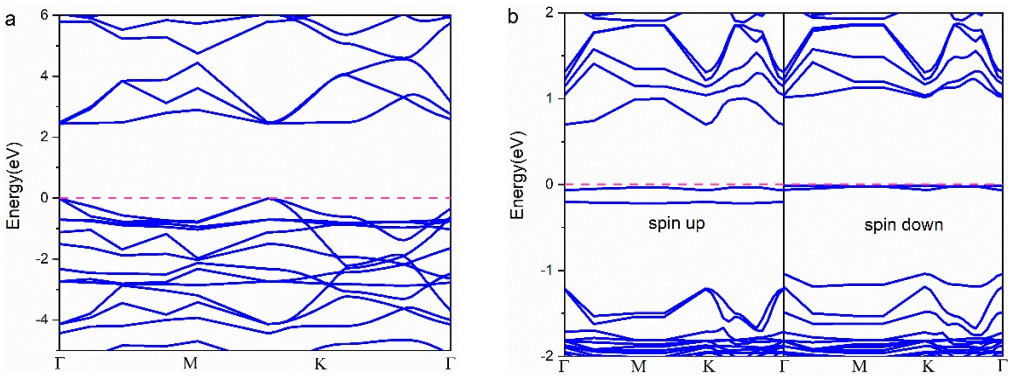

Figure S9. Band structures of (a) pristine C_2N and (b) B-Co@C_2N, where the Fermi levels are set to zero and represented by pink dash lines.

Table S1 Calculated ZPE and TS energies for different species, where the label * denotes the status of adsorption.

Adsorbed species	E_{ZPE} (eV)	E_{TS} (eV)
CO	0.14	0.62
H_2	0.27	0.41
H_2O	0.60	0.59
C_2H_4	1.39	0.69
C_2H_5OH	2.14	0.85
C_2H_6	1.99	0.69
***COOH**	0.66	0.18
***CO**	0.20	0.14
***2CO**	0.42	0.29
***COCO**	0.41	0.26
***COCHO**	0.74	0.24
***COCHOH**	1.07	0.22
***COHCHOH**	1.39	0.23
***CHCOH**	0.94	0.15
***CHCHOH**	1.20	0.17
***CHC**	0.53	0.09
***CH_2CHOH**	1.55	0.19
***CHCH**	0.80	0.10
***CH_3CHOH**	1.84	0.27
***$CHCH_2$**	1.16	0.11
***C_2H_5OH**	2.14	0.34
***C_2H_4**	1.44	0.13
***C_2H_5**	1.74	0.17
***C_2H_6**	2.01	0.29