Supporting information for:

Silicon-Doped Graphene Edge: An Efficient Metal Free Catalyst for the Reduction of CO_2 into Methanol and Ethanol

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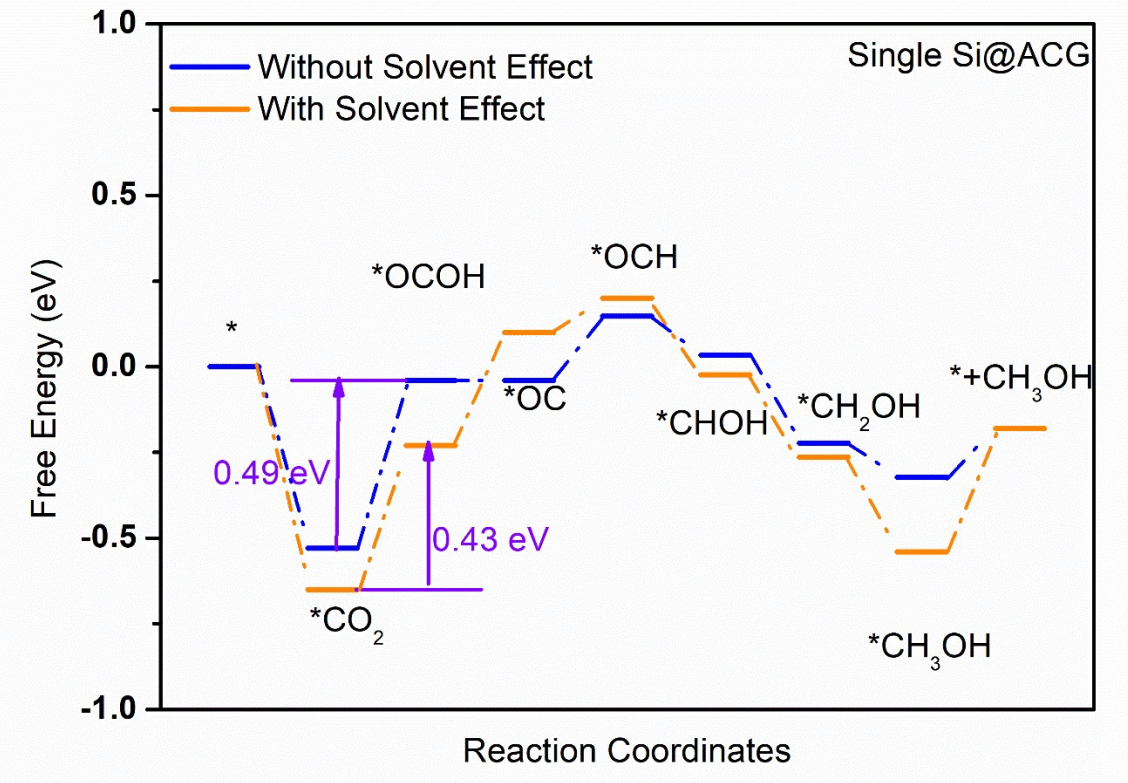

Figure S1. The Gibbs free energy changes for Si@ACG with and without solvent effect.

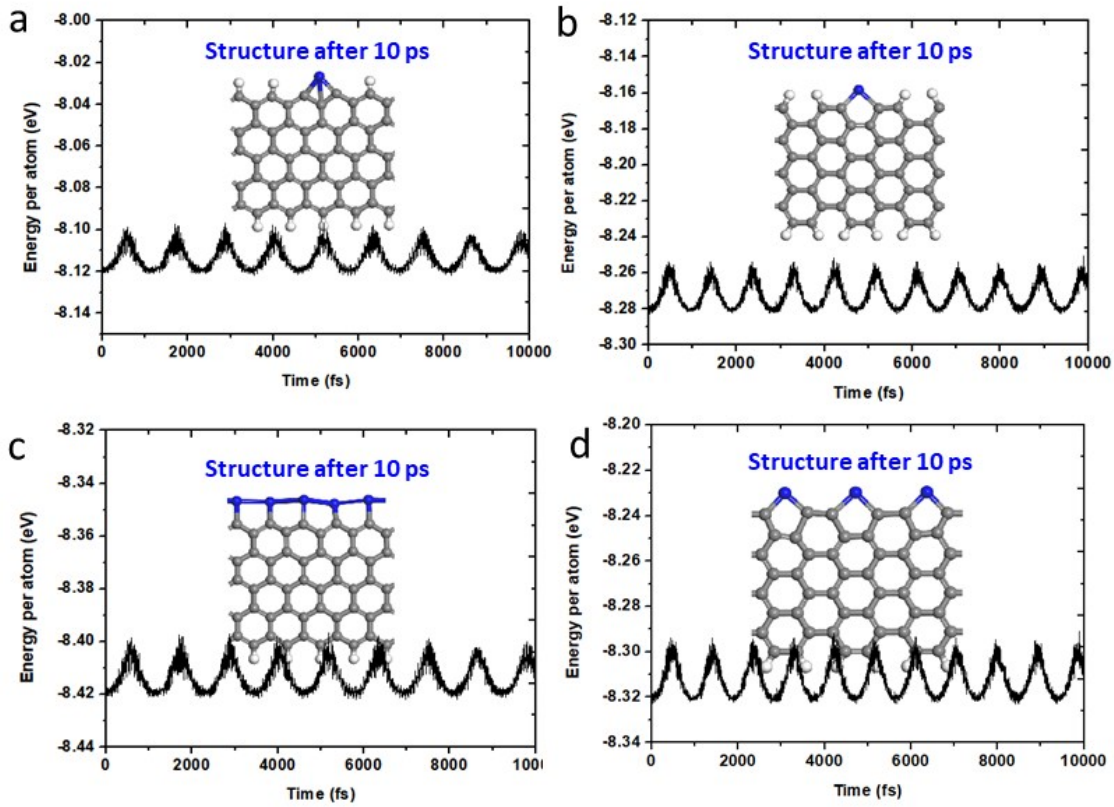

Figure S2. Variations of energy per atom against the time for AIMD simulations for (a) Si@ZZG, (b) Si@ACG, (c) Si chain @ZZG, and (d) Si chain @ACG, insert are the snapshot of the atomic configurations. The simulation is run under 300 K for 10ps with a time step of 1fs.

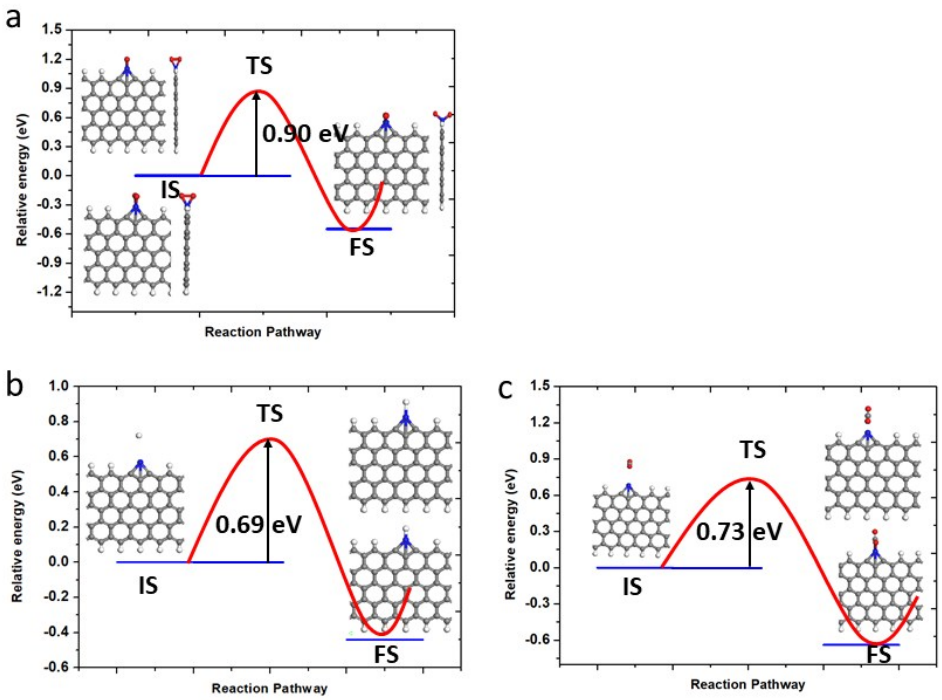

Figure S3. Energy profile for (a) oxidation process of Si @ZZG, (b) adsorption process of H atom, and (c) adsorption process of CO_2 molecule.

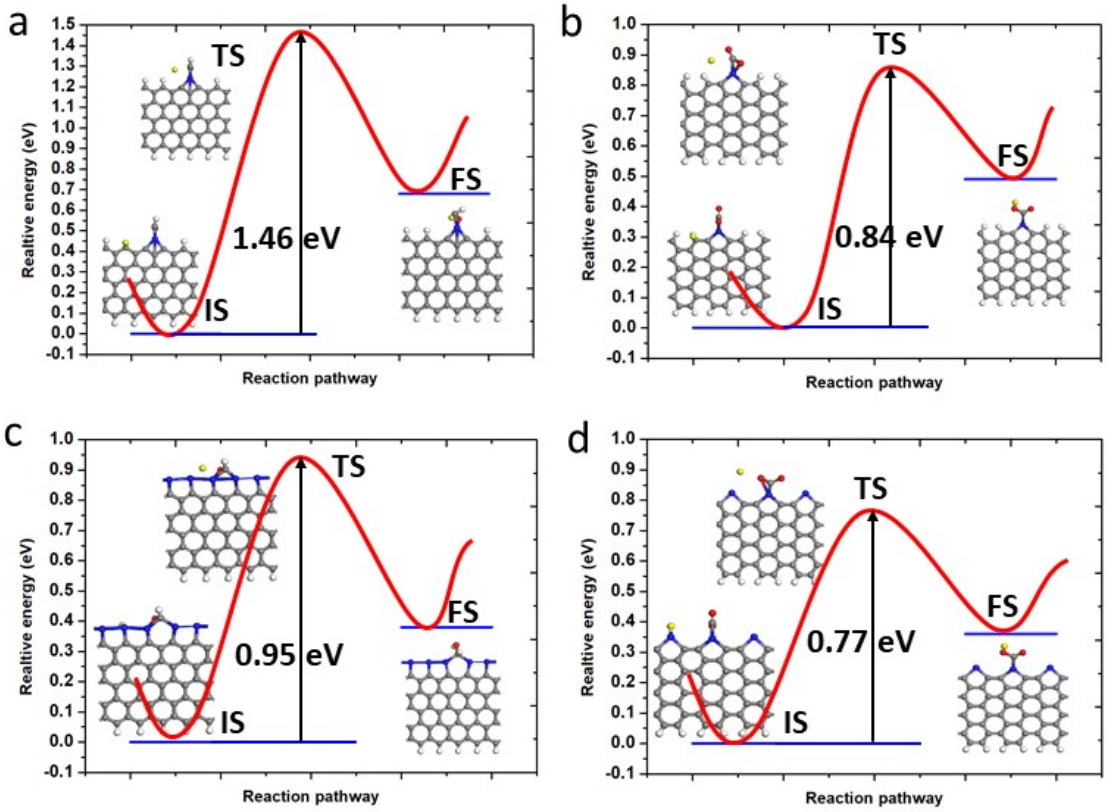

Figure S4. The calculated NEB processes for the formation of CH_3OH on (a) Si @ZZG (PDS: *OCH + *H → *CHOH), (b) Si @ACG (PDS: *COO + *H → *COOH), (c) Si chain @ZZG

(PDS: *OCH + *H → *CHOH), (d) Si chain @ACG (PDS: *COO + *H → *COOH). Insert are the optimised structures for initial structure (IS), transition state (TS), and final structure (FS).

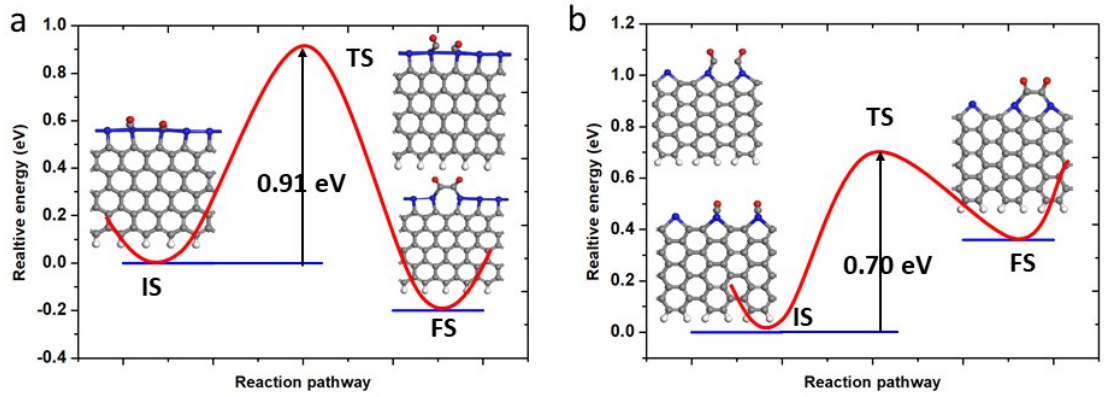

Figure S5. The calculated NEB process for C-C coupling process on (a) Si chain @ZZG, and (b) Si chain @ACG.

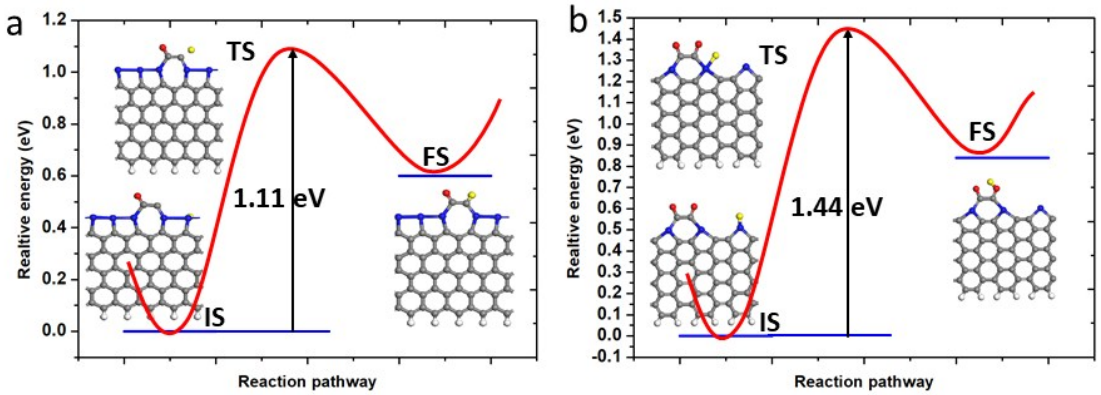

Figure S6. The calculated energy profiles for the formation of CH_3CH_2OH on (a) Si chain @ZZG (PDS: *CCO+ *H → *CHCO), (b) Si chain @ACG (PDS: *COCO + *H → *COCOH). Insert are the optimised structures for initial structure (IS), transition state (TS), and final structure (FS).

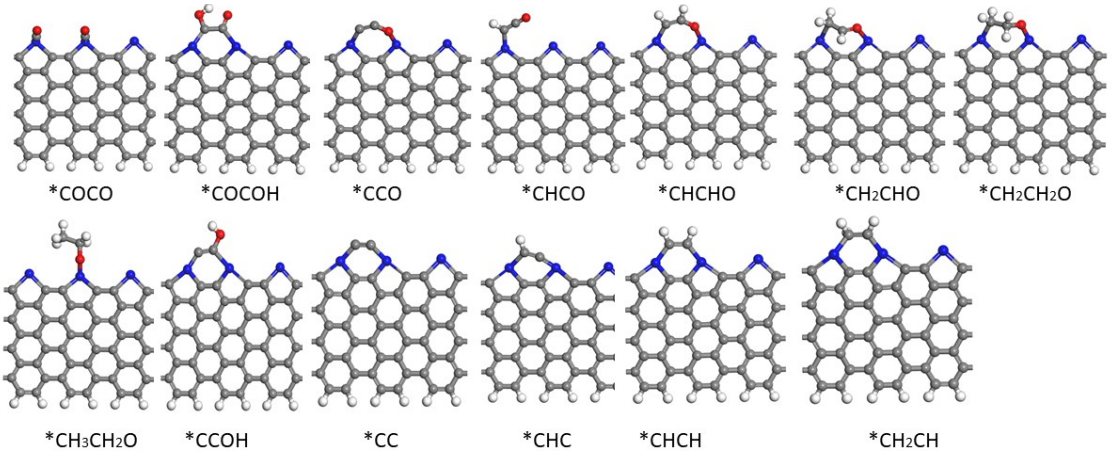

Figure S7. The optimized structures for the intermediates of the CH_3CH_2OH and C_2H_4 formation processes on armchair edge.