Supporting Information

Silica-Confined Two-Atom Single-Cluster Catalyst for Direct Nonoxidative Conversion of Methane: A DFT Study

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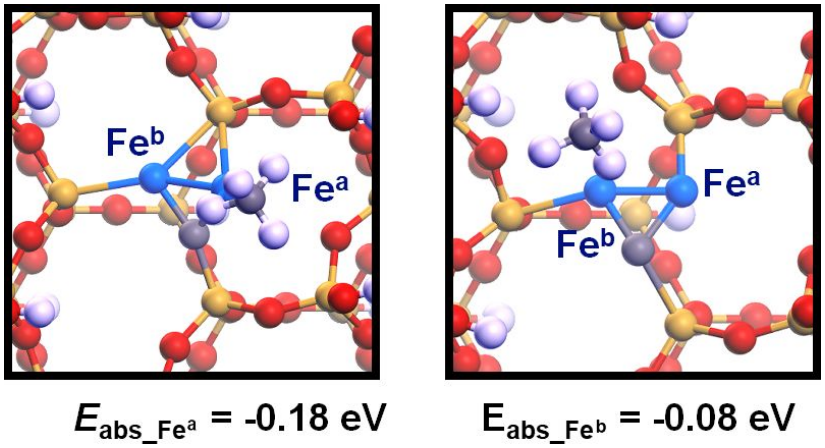

Figure S1. Absorption structure and energy of methane on Fe^a and Fe^b atom of $Fe_2C©SiO_2$.

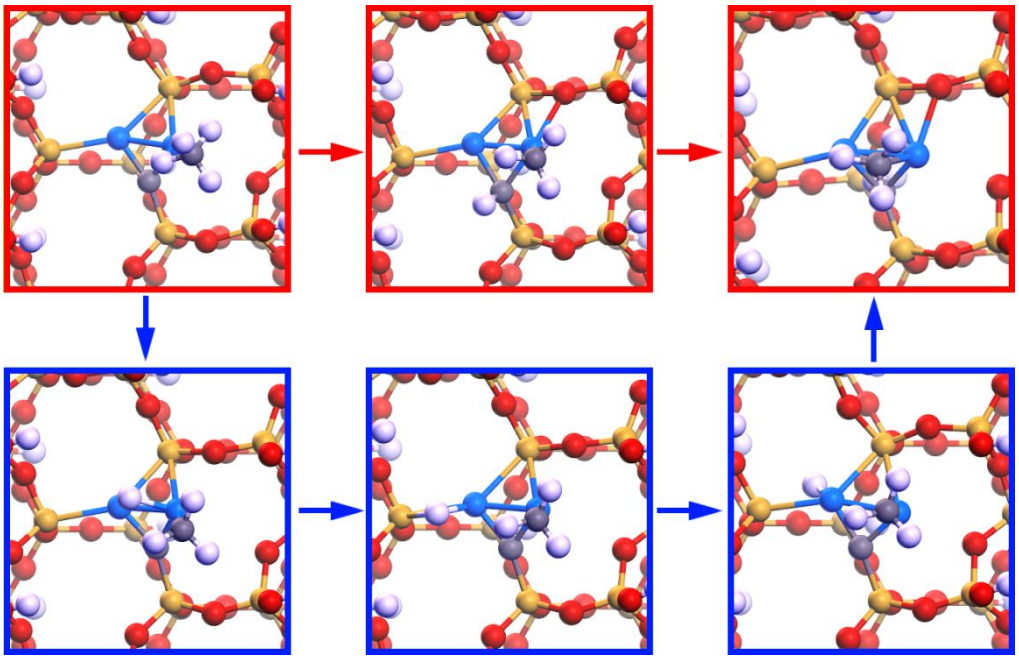

Figure S2. Optimized structures of different reaction paths for the dissociation of methane.

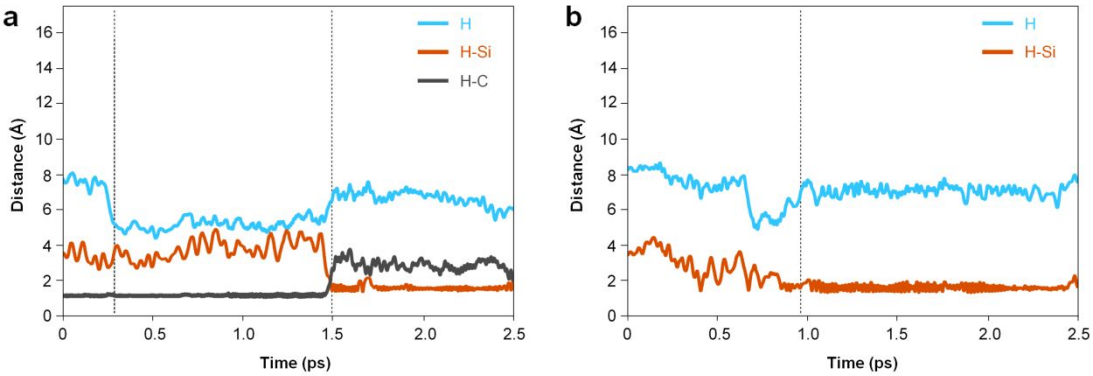

Figure S3. Ab-initio molecular dynamics simulation for the distance of H-Si bond, H-C bond and the *z* coordinate of H atom. The initiating structures are (a) CH_3*+H^d and (b) CH_3* + H^a.

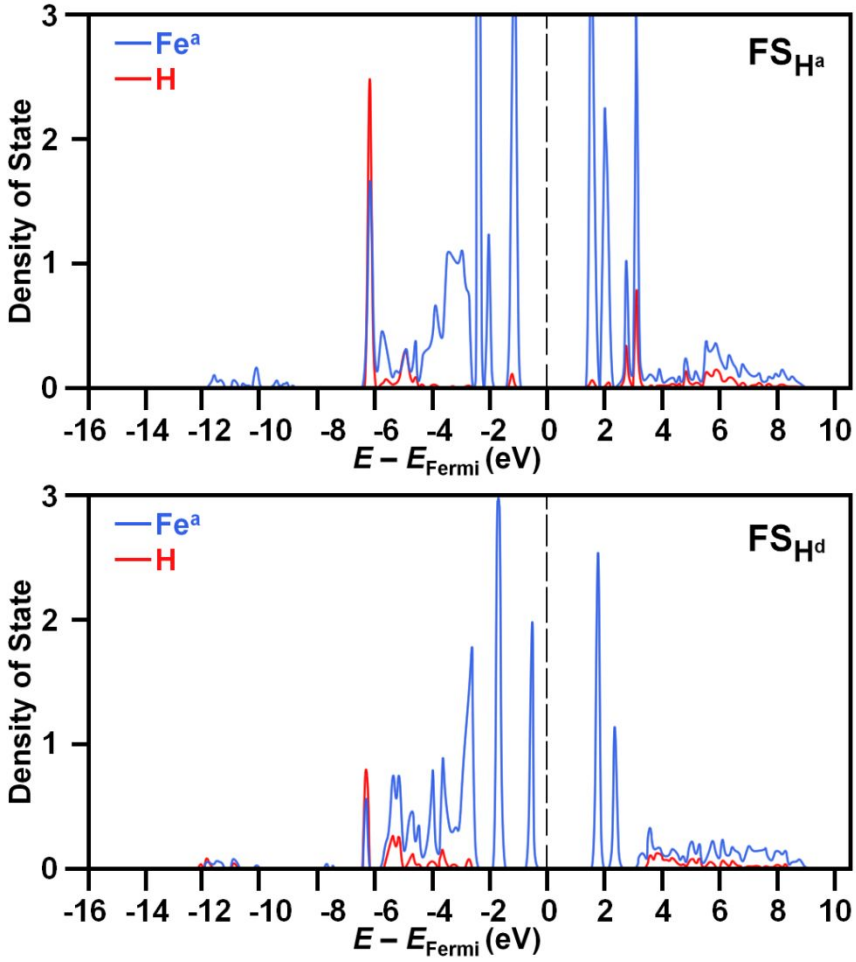

Figure S4. Partial density of states (PDOS) of *d*-band of Fe^a (cyan line) and H (red line).

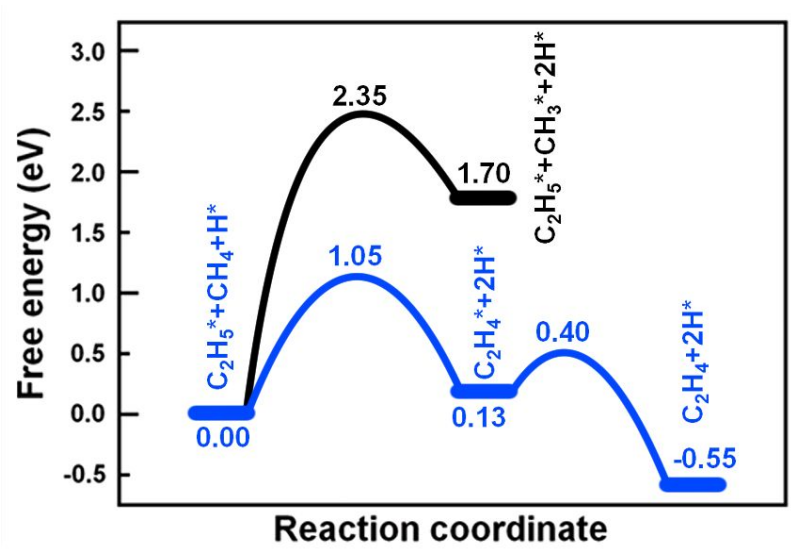

Figure S5. Free energy profiles for the dissociation of the methane with co-adsorption of ethyl (black line) and dehydrogenation of ethyl to ethylene (blue line).

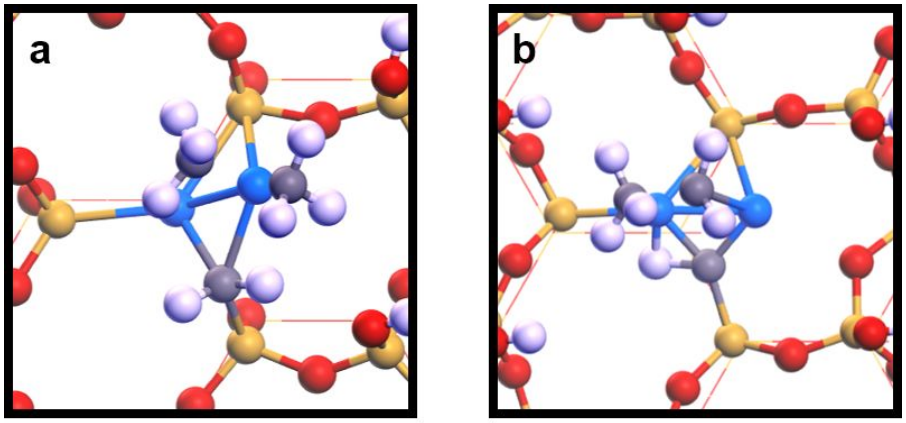

Figure S6. Structures of the transition states for coupling of (a) methyl-methyl and (b) methyl-methylene.

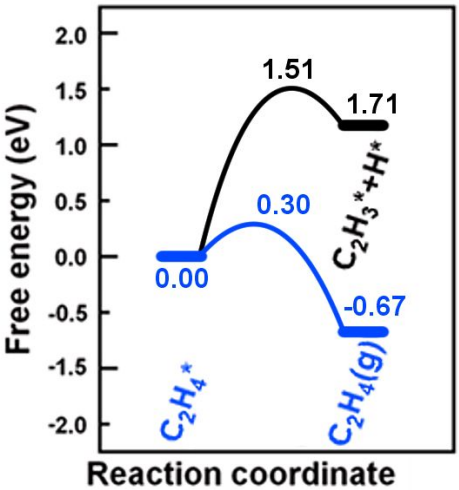

Figure S7. Free energy profiles of the dehydrogenation and desorption of C_2H_4