

Description of Additional Supplementary Files

File Name: Supplementary Data 1

Description: Structures, formation energies, and vibrational frequencies of species used in microkinetic analysis for the non-oxidative methane coupling reaction. Formation energies were calculated using electronic energies of CH₄, H₂, and structure '1.0' as references. Color reference: brown, C; white, H; silver, Si; red, O; gold; Fe.

File Name: Supplementary Data 2

Description: Elementary reactions involved in the microkinetic modelling. * and _g denote surface and gas-phase species, respectively.