Computational-aided design of the catalysts for CH_4 Activation and Conversion

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Despite significant progress in low-temperature methane activation, commercial viability, specifically obtaining high yields of C1/C2 products, remains a challenge. High desorption energy (>2 eV) and overoxidation of the target products are fundamental limitations in CH4 utilization. Herein, we employ first-principles density functional theory (DFT) and microkinetics simulations to investigate the CH4 activation and the feasibility of its conversion to C_2H_4 on the RuO_2 (110) surface with high reactivity (Ea = 0.60 eV)[1]; to H_2 via steam reforming on Ir/RuO_2 (110) surface[2]; methanol on Cu_2O_2 stabilized within MIL-53 (Al) framework[3].

References

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