Highly activated K-doped iron carbide nanocatalysts designed by computational simulation for Fischer–Tropsch synthesis†

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Although the reaction results of numerous iron-based Fischer–Tropsch synthesis catalysts containing various promoters have been reported, the research on their theoretical foundation is still insufficient. In the present work, highly activated K-doped χ-Fe_5C_2/charcoal nanocatalysts were designed using calculations based on density functional theory (DFT), and then prepared using a melt-infiltration process and a subsequent incipient-wetness method of K precursors. The catalyst at K/Fe = 0.075 in an atomic ratio that bears small iron carbide nanoparticles of ~18 nm showed the highest activity (1.54×10^{-4} mol_{CO} g_{Fe}^{-1} s^{-1}) and the best hydrocarbon yield (1.41×10^{-5} g_{HC} g_{Fe}^{-1} s^{-1}), as well as a good selectivity for gasoline-range (C_5–C_{12}) hydrocarbon products in the high-temperature Fischer–Tropsch reaction.