Materials Advances

Electronic Supplementary Information for

Unravelling the K-promotion effect in a highly active and stable Fe_5C_2 nanoparticle for catalytic linear α-olefin production

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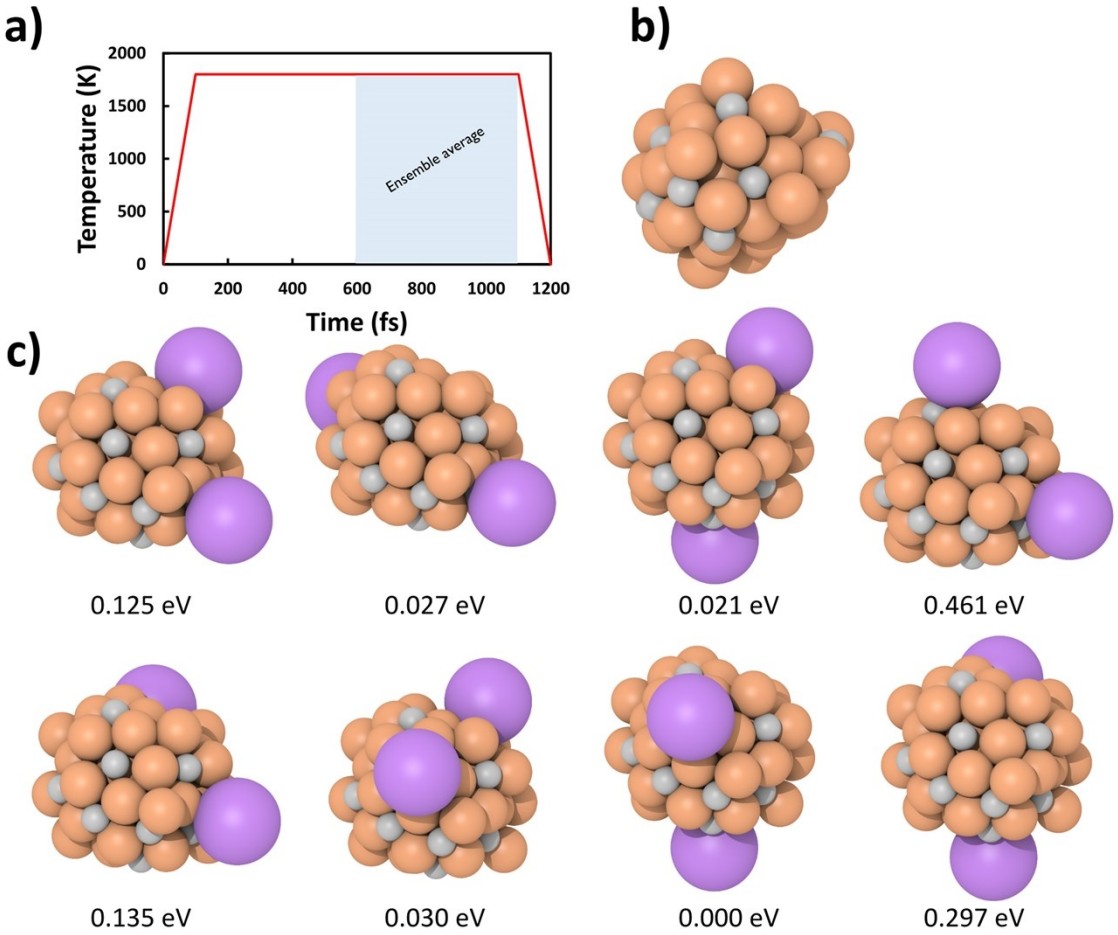

Figure S1. (a) Temperature profile as a function of time in first-principles molecular dynamics simulations for generating a reliable Fe_5C_2 nanoparticle structure. (b) Geometry optimized K-free Fe_5C_2 nanoparticle structure. (c) K-doped Fe_5C_2 nanoparticle structures with different locations of two K atoms and total energy relative to their most stable configuration. Dark orange, grey and purple indicate Fe, C and K atoms, respectively.

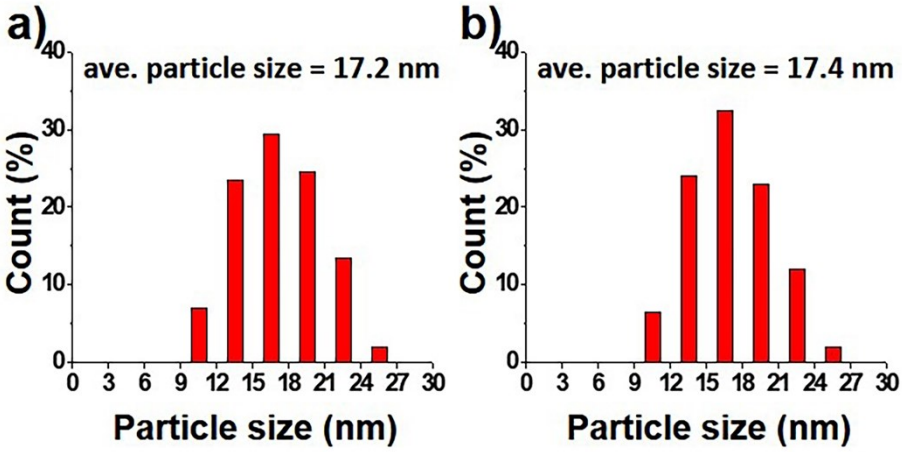

Figure S2. Particle size distributions of (a) K-free Fe_5C_2 nanoparticles and (b) K-doped Fe_5C_2 nanoparticles in each catalyst. More than 200 particles were counted for the sample.

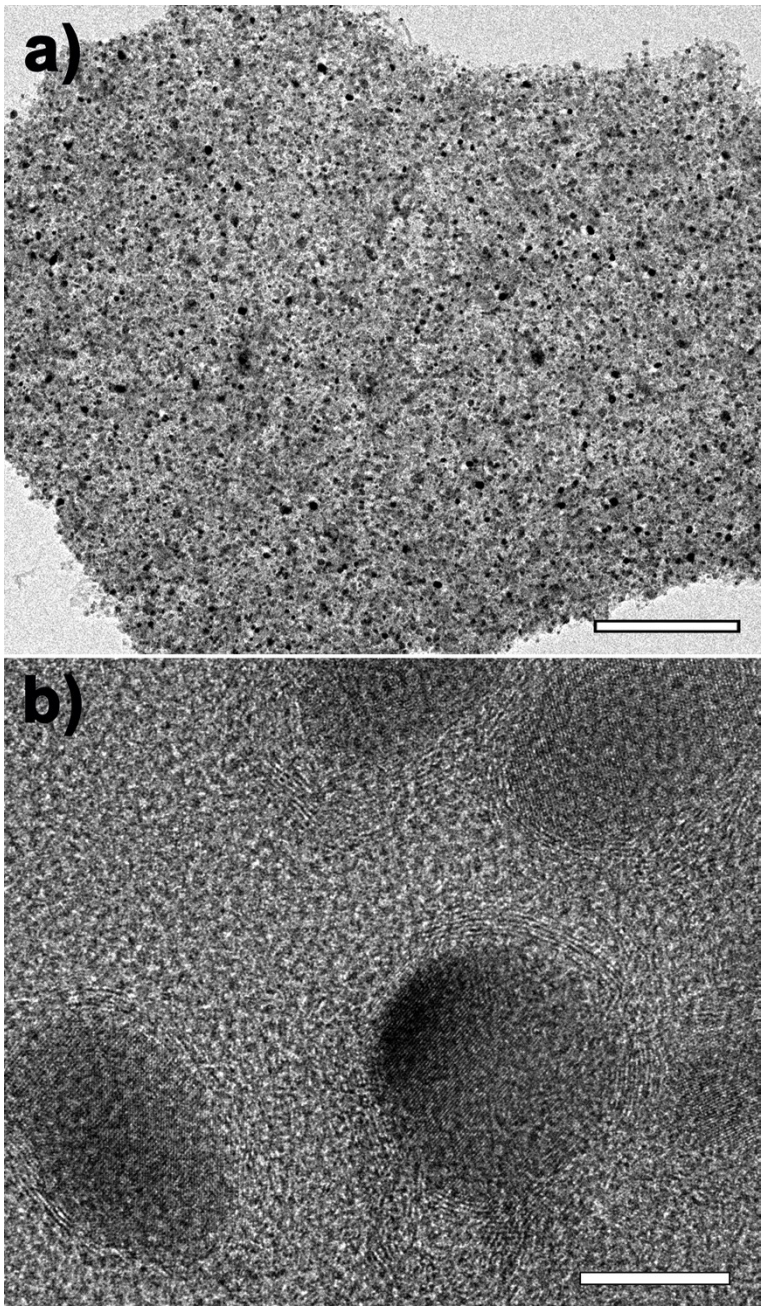

Figure S3. (a) Low-resolution TEM and (b) HRTEM images of the recovered K-Fe_5C_2@C/NPC nanocatalyst after the HT-FTS reaction for 78 h. The bars represent 500 nm (a) and 10 nm (b).

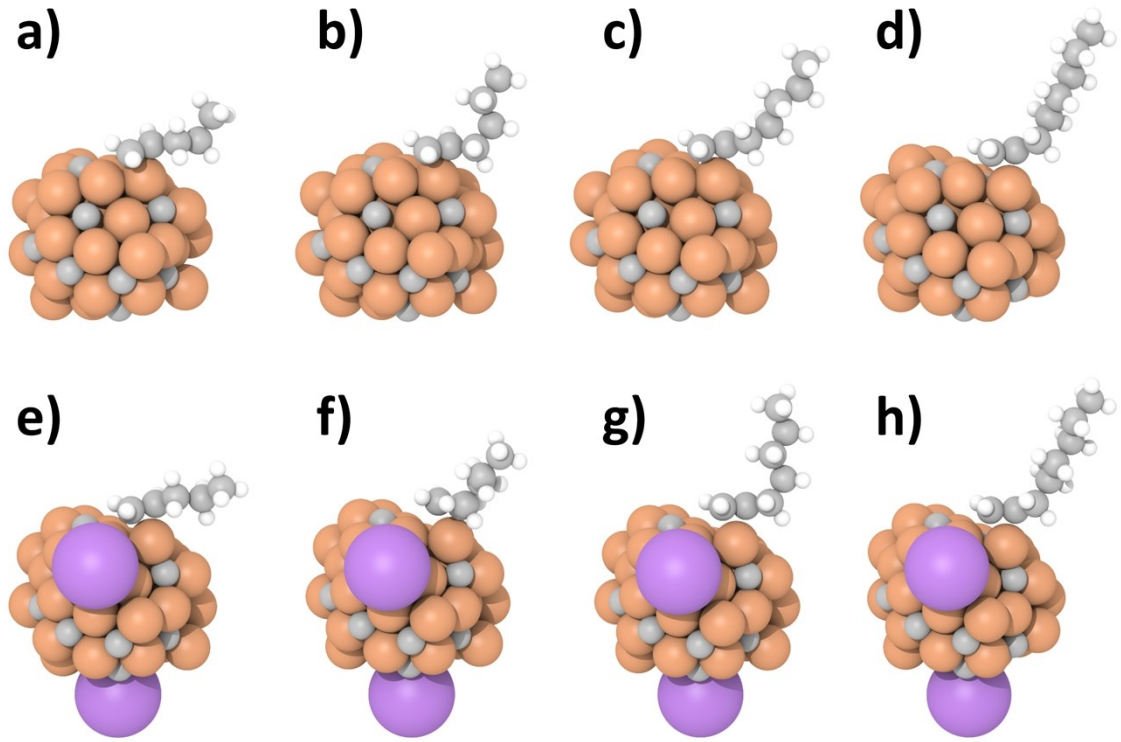

Figure S4. Geometry optimized structures of (a, e) 1-pentene, (b, f) 1-hexene, (c, g) 1-heptene and (d, h) 1-octene on (a-d) K-free Fe_5C_2 nanoparticle and (e-h) K-Fe_5C_2 nanoparticle. Dark orange, grey, white and purple balls represent Fe, C, H and K atoms, respectively.

Table S1. Comparison of the CO conversion and FTY values of the K-doped Fe_5C_2@C/NPC nanocatalyst with those found in the literature for K-doped Fe catalysts to be used under high-temperature Fischer-Tropsch synthesis conditions.

Catalyst	GHSV ($NL \cdot g_{cat}^{-1} \cdot h^{-1}$)	Total CO conv. (%)	FTY ($\times 10^{-4}\ mol_{CO} \cdot g_{Fe}^{-1} \cdot s^{-1}$)	Ref.
K-Fe_5C_2@C/NPC (Fe: 33.7 wt%)	42	96.7	4.4	This work[a)]
K-Fe_5C_2/Charcoal (Fe = 20 wt%)	8	~ 94	1.54	[1][b)]
0.5K-Fe_3C@C (Fe: 22.4 wt%)	15	74.8	2.69	[2][c)]
0.6K38-Fe@C (Fe: 38 wt%)	60	93	4.38	[3][d)]
KFe@C-MIL100 (Fe: 38.1wt%)	60	94.9	4.23	[4][e)]
KFe@C-F300 (Fe: 35.7wt%)		91.7	4.59	
KG16Si (Fe: 16wt%)	3	84.8	0.39	[5][f)]

Catalytic tests were carried out at a) T = 340°C, P = 1.5 MPa, H_2/CO ratio = 1, b) T = 320°C, P = 1.5 MPa, H_2/CO = 1, c)T = 320°C, P = 2.0 MPa, H_2/CO ratio = 1, d)T = 340°C, P = 2.0 MPa, H_2/CO ratio=1, e)T = 340°C, P = 2.0 MPa, H_2/CO ratio = 1. f) T = 340°C, P = 2.0 MPa, H_2/CO ratio = 1.7,

References

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