

Supplementary Material for
**Initial stage of carbonization of iron during hydrocarbons
dissociation: a molecular dynamics study**

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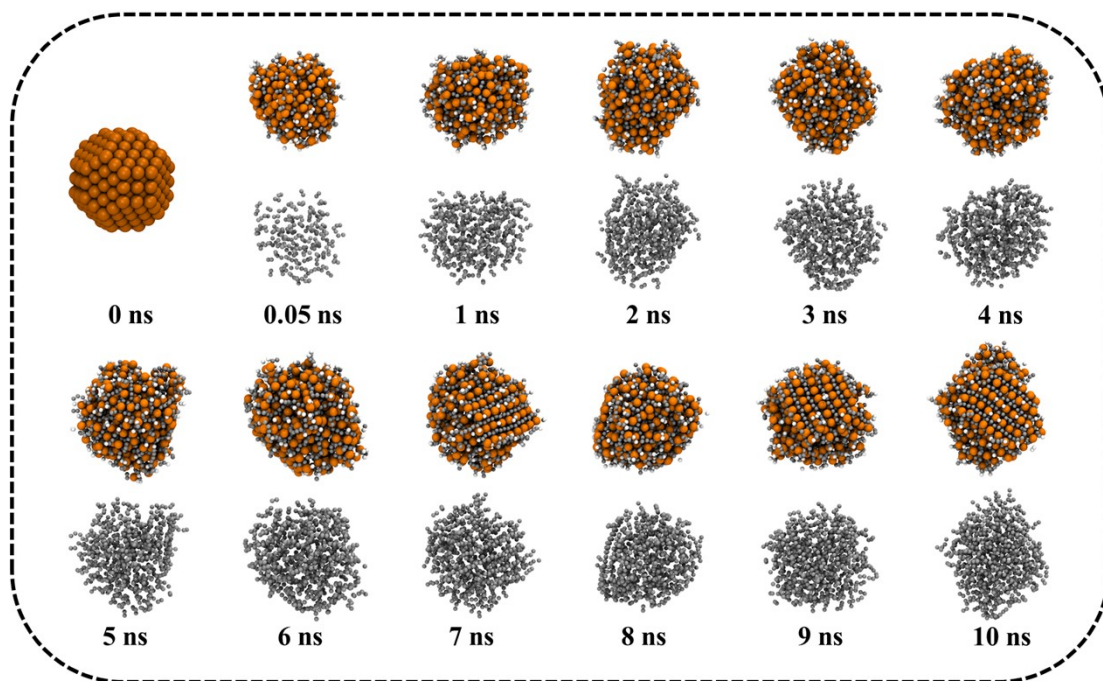


Fig. S1 Morphological evolution of Fe nanoparticles during C_2H_6 dissociation.

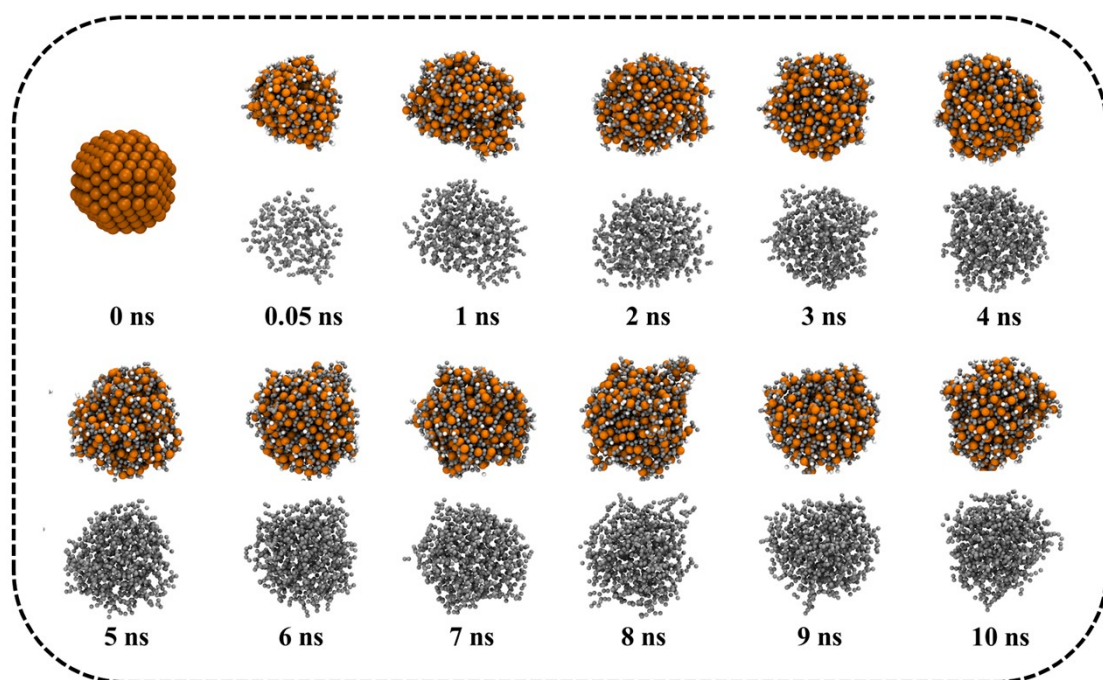


Fig. S2 Morphological evolution of Fe nanoparticles during C_2H_4 dissociation.

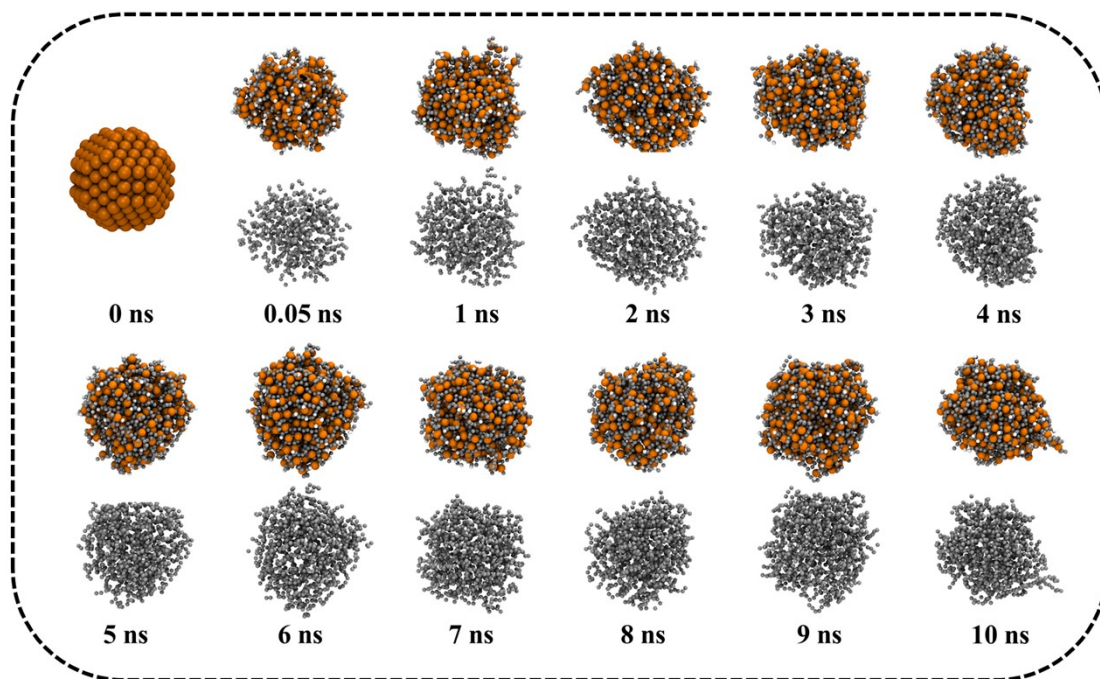


Fig. S3 Morphological evolution of Fe nanoparticles during C_2H_2 dissociation.

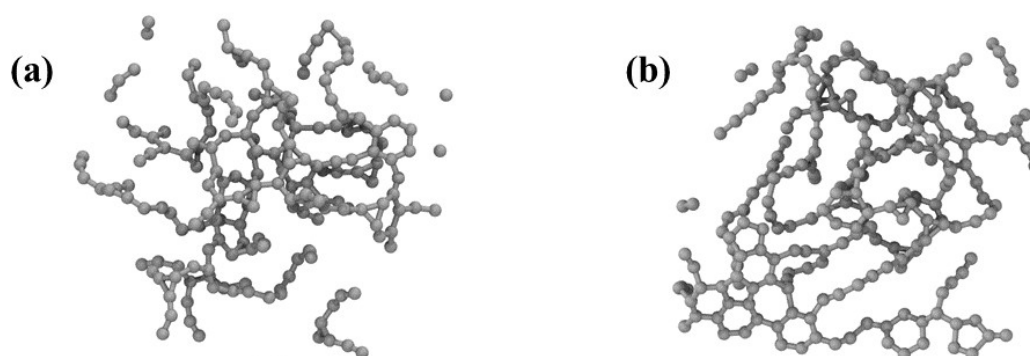


Fig. S4 Local configuration of the carbon chain formed by (a) C_2H_4 and (b) C_2H_2 at 10 ns reaction time.

Table S1. Density of carbon atoms (g/cm^3) in Fe nanoparticles after the reaction.

	CH_4	C_2H_6	C_2H_4	C_2H_2
Density	2.19	2.33	2.56	2.86