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Phase diagrams for Fe-C nanoparticles: A Molecular Dynamics Study[1] NEHA AWASTHI, AIQIN JIANG, ALEKSEY KOLMOGOROV, Duke University (USA), FENG DING, Rice University (USA), KIM BOLTON, Goteborg University (Sweden), ELENA MORA, Ohio State University (USA), TOSHIO TOKUNE, AVETIK HARUTYUNYAN, Honda Research Institute (USA), STEFANO CURTAROLO, Duke University (USA) — Fe nanoparticles are widely used as catalysts for carbon nanotube growth. In order to better understand the melting and phase transition properties of these nanoparticles, molecular dynamics (MD) simulations are performed to determine the melting point of Fe-C nanoparticles ($\sim$ 1- 4 nm size) as a function of size and carbon concentration. The temperature dependence of the total energy and the Lindemann index characterize the melting of nanoparticles. For free (unsupported) Fe-C clusters, it is observed that the eutectic point (in the phase diagram) shifts with nanoparticle size. We have investigated how the presence of a substrate affects the melting process of the Fe-C nanoparticles.

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