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Fe on graphene: interaction, growth morphology, and thermal stability XIAOJIE LIU, Beijing Computational Scientific Research Center, Beijing, 100084, People's Republic of China, CAI-ZHUANG WANG, MYRON HUPALO, Ames Laboratory-US Department of Energy, and Department of Physics and Astronomy, Iowa State University, Ames, Iowa, 50011, USA, HAI-QING LIN, Beijing Computational Scientific Research Center, Beijing, 100084, People's Republic of China, KAI-MING HO, MICHAEL TRINGIDES, Ames Laboratory-US Department of Energy, and Department of Physics and Astronomy, Iowa State University, Ames, Iowa, 50011, USA — The nucleation and growth of Fe on graphene is highly unusual. Constantly increasing in island density with coverage is observed by experiment which indicates the presence of strong adatom predominantly repulsive interactions. We study Fe adatoms interactions on graphene by first-principles calculations and showed that the interactions between Fe adatoms consist of a short-range attraction and long-range repulsions. By investigating the adsorption energies and diffusion barriers for Fe adatoms on graphene, we also predict that Fe on graphene exhibit a three-dimensional growth mode. Fe nanostructures on graphene are also shown be stable against aggregation. The predictions from first-principles calculations are consistent with experimental observations.

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