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Interstitial Functionalization in elemental Si BORIS KIEFER, EDWIN FOHTUNG, New Mexico State University — Societies in the 21st century will face many challenges. Materials science and materials design will be essential to address and master some if not all of these challenges. Semiconductors are among the most important technological material classes. Properties such as electrical transport are strongly affected by defects and a central goal continues to be the reduction of defect densities as much as possible in these compounds. Here we present results of interstitial Fe doping in elemental Si using first-principles DFT calculations. The preliminary results show that Fe will only occupy octahedral interstitial sites. The analysis of the electronic structure shows that the compounds are ferromagnetic and that a bandgap opens as interstitial Fe concentrations decrease, with a possible intermittent semi-metallic phase. The formation energy for interstitial Fe is unfavorable, as expected, by ˜1.5 eV but becomes favorable as the chemical potential of Fe increases. Therefore, we expect that biasing the system with an external electrical field will lead to the formation of these materials. Thus, our results show that interstitial defects can be beneficial for the design of functionalities that differ significantly from those of the host material.

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