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Vacancies and Silicon Defects in Silicene SHUANG LI, None — Structural defects,which may appear during growth or processing, can be used to tailor the local properties and to achieve new functionalities. Reconstruction of silicene with vacancies formed by up to six missing atoms, rotated defects and adatoms are investigated using a first-principles electronic-structure study in the framework of density-functional theory. The local structures of defects, their stability and electronic structure are discussed. We found that defects in silicene can induce structural reconstruction, and some of these reconstructions can open a band gap, which is of importance when building nanoelectronic devices.

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None

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