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Intrinsic defect interactions in a monolayer silicene: An ab-initio DFT study

Tuesday, 4 July 2023 16:00 (1 minute)

Silicene is a two-dimensional structure of silicon which has been synthesized experimentally. It is mechanically and thermally stable and possess the possibility of being easily integrated into the existing silicon technology, hence its importance in semiconductor device technology. However, the performance of any semiconductor material is dependent on the type, stability, and interactions between the defects as well as the mobility of defects that are intrinsic to it. Using the density-functional theory (DFT) approach, we study the stability, electronic and magnetic interactions between various vacancy defect configurations in silicene. We provide a deeper understanding of fundamental properties of defective silicene containing vacancies and also demonstrate how the presence of vacancy-like defects may impact on the potential applications of silicene in such fields as spintronics and valleytronics.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

PhD

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