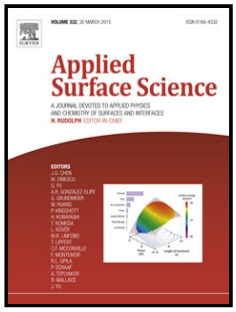

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First-principles calculations study of *Na* adsorbed on silicene

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Abstract

Geometry, electronic structure, and diffusion properties of *Na* atom on the pristine and single vacancy-defected silicene sheet have been systematically investigated by using density functional theory with generalized gradient approximation. The most stable positions of *Na* atom on the perfect and the defected silicene sheet are determined, and four diffusion paths have been explored. The minimum diffusion barrier of *Na* atom is 0.25eV on pristine silicene, and 1.44eV on single-vacancy defect silicene sheet. The vacancy exhibits a more significant influence than the adsorption of *Na* atom on the electronic structure of silicene.

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