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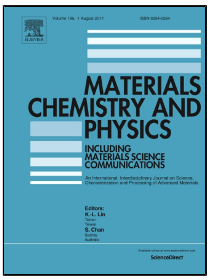

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Oxygen defects formation and optical identification in monolayer borophene

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Abstract

Surface reactions with oxygen are a fundamental cause of the degradation of borophene, which has greatly limited the application in nanoelectronic and optoelectronic devices. Density functional theory calculations disclose that there is an energy release of about 3 eV for each oxygen atom adsorbed onto borophene. The hybridization between p_z orbitals of oxygen and p orbitals of neighboring B atoms lead to minor distortions of the lattice and low energy metastable forms, finally to form different oxygen defects. The mechanism for oxidation involving reactive dangling oxygen atoms is proposed, and absorption spectra are suggested to identify the types of oxygen defects in borophene.

Keywords: Oxygen defects; First-principle calculation; Monolayer borophene

PACS: 73.20.At; 73.30.+y; 74.78.Fk

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