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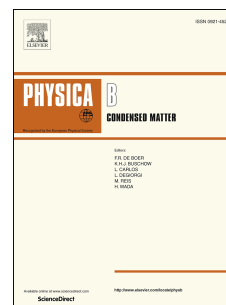
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The adsorption and dissociation of oxygen on Ag (111) supported χ_3 Borophene

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Abstract: The superstructure of χ_3 borophene on Ag (111) has recently been synthesized in experiment. In this work, we investigate its structural, electronic properties and the oxidation mechanism through first-principles calculations. We find the superstructure of χ_3 borophene on Ag (111) maintain the planar characteristics, like its free-standing form, owing to the weakly interaction between adsorbate and substrate. Moreover, oxygen molecule can be spontaneously adsorbed on its superstructure in a manner of chemical adsorption. Importantly, the energy barrier of ~ 0.35 eV for oxygen dissociation indicates its relative stability in ambient conditions compared with the active silicene. Furthermore, the mobility of O_2 -dissociation-induced O atom is poor at room temperature, implying the difficult migration of O atom on borophene surface. On the other hand, due to the strong B-O

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