Physico-Chemical nanomaterials science

Understanding from first principles of the mechanisms of icesolid adhesion

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The formation of ice on surfaces can be a serious problem. Creating anti-icing surfaces requires a thorough understanding of the mechanisms of ice-solid adhesion. However, the fundamental physics of ice adhesion are not yet well understood [1,2]. The present study aims to understand the difference in adhesion strength between ice and hydrophobic or hydrophilic surfaces. We theoretically designed contacts between ice and hydrophobic graphene and hydrophilic aluminum at the atomic level (Fig.1). The values of adhesion and interatomic forces of interaction at the interface between ice and a solid body were studied using our own software complex that implements the zone-structure problem using the method of the electron density functional and the pseudopotential [3].

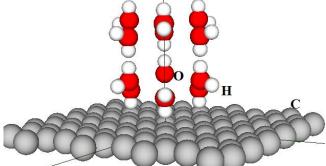


Fig.1. Ice crystal on the surface of graphene

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