

Abstract Submitted
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Electronic and Magnetic Structures in 2D Graphene and BN Nanoflakes¹ WEI-MING SHI, MING JIANG², Department of Physics, Yantai University — The two-dimensional nanomaterials have been attracting great attention for potential applications. Using first-principles calculations, we have studied the geometric and electronic properties of zigzag graphene nanoflake(ZGNF)and single-layer BN nanoflake (ZBNNF)before and after hydrogen and oxygen adsorption. The interplay between atomic adsorption, crumpling structures, zigzag edges and magnetic structures has been investigated systematically. Our calculated results show that the total magnetic moments of the ZGNF with the adsorbed atoms increase significantly. The adsorbed atoms induce the crumpling structures and central spin polarization, while the magnetic orders of zigzag borders are controlled. A detailed electronic structure analysis is given. The single-layer BN nanoflake has a special crumpling struture different from the ZGNF. The left-right symmetry of atomic height displacements is broken. This study demonstrates a new approach to manipulate the properties of 2D nanomaterials. This work was supported by the SRFROCS,SEM and Shandong OYS Foundation.

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