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Theoretical Study on the Structures, Electronic and Magnetic Behaviors of Novel Composite Nanosystems by Adsorbing Superhalogen on the Low-dimensinal BN Structures

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Hexagonal boron nitride (h-BN) can exhibit the fascinating physical and chemical properties, and can be considered as the powerful building block to construct new composite nanomaterials. In this work, by means of the first-principles calculations, we design a new class of composite nanosturcures by adsorbing superhalogen on the surface of low-dimensional BN nanomaterials. The considerably large adsorption energies indicate that the superhalogen can be stably adsorbed on the surface of the BN materials. Independent of dimension, chirality and adsorption site, depositing superhalogen can endow these hybrid BN nanomaterials with a large magnetic moment, and evidently narrow the robust wide band gap of BN materials. Overall, all these new superhalogen-BN composite nanostructures can present the large magnetism and an appropriate band gap, which is very promising to make them an practical application in the field of multifunctional nanodevices in the near future.

Biography

Dr. Xuri Huang received his Ph.D degree from Jilin University in China in 1991. He is currently a full professor and also is the first deputy director in institute of theoretical chemistry, jilin university, China. His research interests mainly focus on the theoretical study on the structures and properties of novel low-dimensional nanomaterials, such as one- or two-dimensional C, BN and SiC nanomaterials.

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