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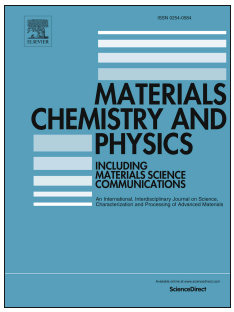

Waved graphene: Unique structure for the adsorption of small molecules

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Waved graphene: unique structure for the adsorption of small molecules

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Abstract: We propose waved graphenes for the strong adsorption of molecules and investigate their potential applications. We find that the physical adsorption of molecules on waved graphene is greatly enhanced by compression. At optimal compression, the physical adsorption energies of H_2, N_2, NO, and CO are increased by 6~9 times, and that for O_2 is more than 2 times. We show that the energy for their chemical adsorption on waved graphene decreases dramatically with the increment of compression. The energy of chemical adsorption and dissociation of H_2 on flat graphene is 1.63 eV and reduced to 0.06 eV (96 % reduction) on waved graphene at a compression of 50 %. The energy for chemical adsorption of O_2 on waved graphenes is extremely reduced from 0.98 eV to -0.57 eV as with compression increasing from 0 to 50 %, indicating the transition of endothermic chemical adsorption to exothermic. We further show that the electronic properties of waved graphenes are modified, leading to the change of electrical characters. We see that the waved graphenes may find applications in gas storage, sensor and catalyst because of enhanced physical and chemical adsorption and the induced change of electronic properties.

Keywords: molecule adsorption and dissociation; waved graphenes; catalysis; first-principles calculation

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