ELECTRONIC PROPERTIES OF FUNCTIONALIZED GRAPHENE NANORIBBONS

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S u m m a r y

Distributions of valence electron density in and the electron energy spectrum of graphene nanoribbons covered with hydrogen, fluorine, or oxygen atoms have been calculated *ab initio* in the framework of the density functional and pseudopotential theories. The emergence of a forbidden gap for graphene nanoribbons with zigzag edges and 9.23 Å in width and its absence in an unconfined graphene plane are shown. The forbidden gap is demonstrated to decrease, as the graphene nanoribbon width increases. For graphene nanoribbons with hydrogen-decorated edges, the energy gap disappears. The interaction between a hydrogen atom and carbon atoms in the graphene nanoribbon plane that are coordinated in accordance with the sp^2-hybridization is shown to induce local changes of the hybridization to the sp^3 type.