Effect of Ringlike Carbon Cluster Deposited on Graphene on Hydrogen Chemisorption

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Chemical properties and ideal structure of graphene can be disrupted by various ways, such as by the producing the vacancies and by the replacement of carbon atoms with other atoms, in particular, with nitrogen or silicon atoms [1]. Ability of graphene to chemisorption depends on the curvature of the graphene also [2]. In our work, changes of ability of a rectangular nanographene ribbon consisting of 272 atoms to chemisorption of hydrogen as a result of its interaction with ringlike carbon clusters have been studied.

Using the second-generation of Brenner interatomic potential [3], the interaction of ringlike carbon clusters with nanographene has been simulated on the basis of energy minimization method. The figure shows the simulation result of the deposition of ringlike 12-atom cluster on graphene. Then, in the same manner, interaction of a single hydrogen atom with different atoms of the nanographene, on which the ringlike cluster is deposited, was simulated. It was found that due to the deposited ringlike cluster cohesive energy of chemisorbed hydrogen is changed to 15% compared to the case of ideal graphene.

The results of computer simulations, the various structural changes and modifications of nanographene ribbon caused by the interaction of ringlike clusters and hydrogen chemisorption will be presented and discussed.

References

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Figures

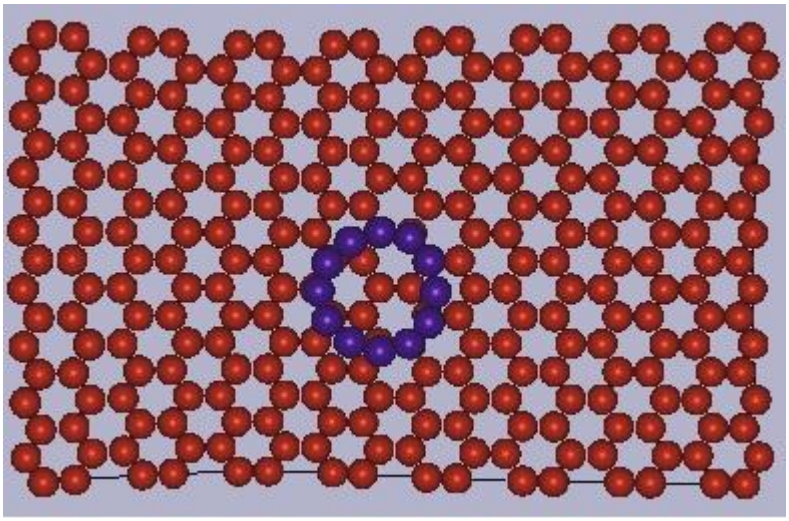

Figure. Ringlike 12-atom carbon cluster (shown in blue) deposited on 272-atom nanographene (shown in red).