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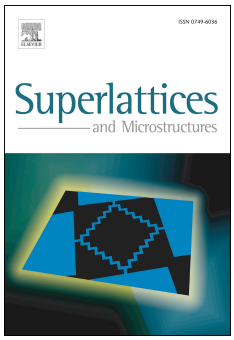

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The effects of metal-cluster on electronic transport of graphene with vacancy studied by first-principles

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ABSTRACT: The configurations of Ag_n (n=1-6) clusters adsorbed at the single and double vacancies of graphene were obtained by density functional theory, and the effect on the electronic transport was studied by non-equilibrium Green's function. It was shown that the conductance of graphene with the clusters adsorbed at the vacancies (concentration of 0.8 at%) increases monotonically with the adsorption energy, which oscillates as 'n' increasing from 1 to 6, and the conductance of the defective graphene can be improved by more than 20% (or 50%) if some of the clusters are adsorbed at the vacancies.

***Keywords*:** graphene; metal adsorption; conductance

1. Introduction

Since graphene [1-3] was first reported, it has been considered to be an ideal material for future high-performance electronic device applications. Electronic transport properties of graphene, as a one-atom thick crystalline material, are sensitive to the presence of atoms adsorbed on its surface. In particular, metal atom adsorption on graphene sheet has attracted considerable attentions for years [4-17]. Previous theoretical studies showed that metal adatoms on graphene surface serving as scattering centers (charged impurities) led to a decrease of graphene conductivity while clustering of the adatoms increased the suppressed conductivity [11-13], which was qualitatively consistent with some followed experimental results [14-17].

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