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Effect of edge vacancies on localized states in semi-infinite zigzag graphene sheet

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Localized zero-energy edge electronic states were theoretically predicted in graphene ribbons and semi-infinite sheets with a crystallographically clean zigzag-type termination [1–4]. These states are characterized by a high electronic density (DOS) at the Fermi level and robustness to weak external perturbations. Edge states are expected to play a notable role in graphene nanoelectronic applications providing a specific tunneling current in graphene-based tunnel junctions [5, 6]. Vacancies are appeared during the synthesis of graphene [7] and being located on the edge atoms of graphene sheet can affect the stability of edge states. This influence will change the main characteristics of nanoelectronic devices operating on the basis of tunnel current through these states. In this work, we study the influence of both the concentration and different location of edge vacancy defects on the stability of edge states in zigzag-type semi-infinite graphene sheet. Three types of distributions have been considered: normal, uniform, and periodic. The calculations are performed by using the Green's function method and the tight-binding approximation. Defects are positioned in graphene sheet by making use of a random number generator. Each atomic position is assigned a weighting factor in accordance with either normal or uniform distribution. In the case of periodic distribution, single vacancies are located with the period of one and two atoms. We have specified the number of atoms between edge vacancies (r). When vacancies are located at a distance of one or two atoms, their mutual influence leads to the appearance of subpeaks in the LDOS (Fig. 1a). In this case, LDOS becomes redistributed between subpeaks and the edge state: the peak near the Fermi level decreases while subpeaks increases. Such behavior does not occur in the case of vacancies without interference (three and more atoms between vacancies). The edge state turns out to be destroyed most effectively when vacancies are located

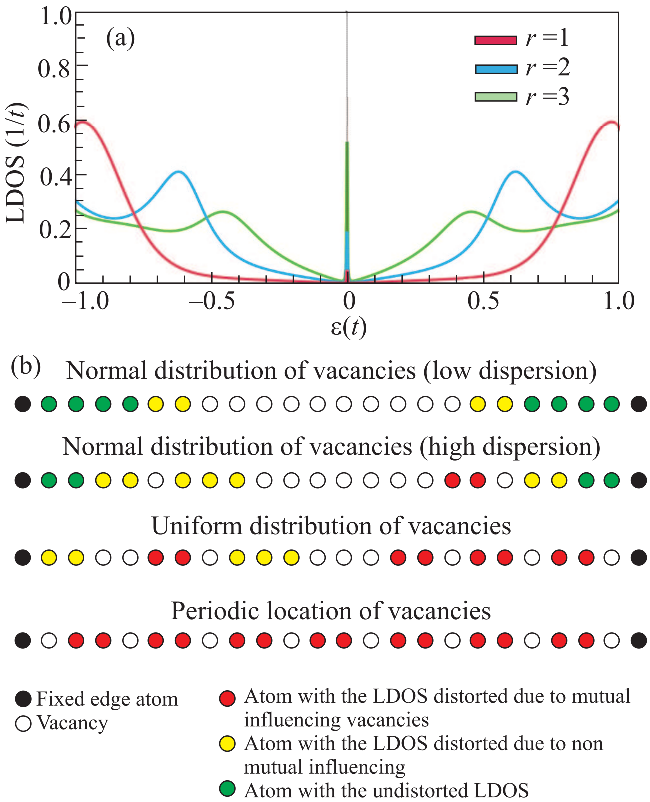

Fig. 1. (Color online) (a) – LDOS of edge atoms located between two single vacancies for different r (the number of atoms between vacancies). Subpeaks are associated with the presence of defects. (b) – An illustrative picture of the LDOS at edge atoms for different vacancy distributions. The edge state disappears when LDOS is distorted at all atoms (for two bottom chains)

at a distance not exceeding the characteristic range of mutual influence (Fig. 1b). The more vacancies influence each other, the lower concentration of defects needed to destroy the edge state. The results of our study may be summarized as follows: (i) when vacancies are located according to the normal distribution, the edge state is degraded at high concentration of defects (more than

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70 %); (ii) for the uniform distribution, the edge state is found to disappear at smaller but nevertheless quite large concentrations exceeding 50 %; (iii) the edge state disappears for single vacancies distributed with the period of one and two atoms. This corresponds to a 30 % vacancy concentration and higher. The stability of edge states depends critically on the position of defects and can only be ensured in the case of 30 % and lower vacancy concentration. However, it should be taken into account that arising subpeaks may affect the performance of molecular devices.

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