

## Stability and Dynamics of Defects in Graphene: Combinatorial Study of HR-TEM and Simulation methods

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### Abstract

Defects in graphene have become a subject of intensive investigation because those affect the mechanical and electronic properties of graphene. In order to observe and control the defects in graphene, many state-of-the-art techniques such as high resolution transmission electron microscopy (HR-TEM) have been devoted to the study of the structure and formation process. However, it is very difficult to observe the detail of the formation process even within the state-of-the-art microscopy methods because the dynamics of defective structures such as vacancy, adatom, and edge atoms is completed in very short time. Various simulation methods have been employed to elucidate the hidden process of defect formation and dynamics [1]. In the study of defect formation and dynamics in graphene, we performed the cooperative research of HR-TEM and simulation methods. In the simulation methods, we used the tight-binding molecular dynamics simulation and density functional theory (DFT) calculation.

In this study, it is found the hydrogen-free graphene edges and our TBMD simulation results are in excellent agreement with images from HR-TEM. These results are expected to make an effective way toward the functionalized graphene [2]. We also found from tight-binding calculation and HR-TEM study that the dislocation core with pentagon-heptagon pair originates ripples which are an out of plane distortion that help stabilize suspended monolayer graphene [3]. We also show that the introduction of atomic vacancies in graphene disrupts the uniformity of C-C bond lengths immediately surrounding linear arm-chair defects in graphene. The measured changes in C-C bond lengths are related to DFT calculations of charge density variation and corresponding DFT calculated structural models [4]. If time allows, we will introduce briefly our recent results on metal dopants in graphene which show interesting results on magnetic property.

### References

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## Figures

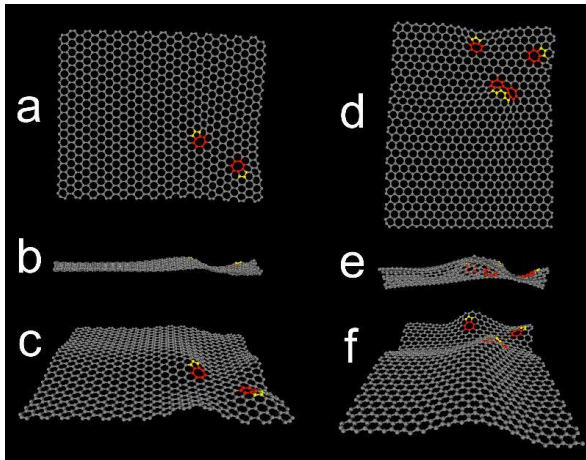


Figure 1. Simulation of ripples in graphene from dislocation addition and their analysis. (a)-(f) Atomic models obtained from tight-binding calculations of graphene (top, side and 3D views) for (a)-(c) two dislocations and (d)-(f) four dislocations.

