Defects in Two Dimensional Materials: Cooperative Study of HR-TEM and Simulation

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Abstract

Defects in two dimensional materials have become a subject of intensive investigation because those affect the mechanical and electronic properties of materials. In order to observe and control the defects, many state-of-the-art techniques such as aberration corrected transmission electron microscopy (AC-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, the tight-binding molecular dynamics simulation and density functional theory (DFT) calculation are employed. From the cooperative research, we found the hydrogen-free graphene edges [2], the stability and dynamics of tetravacancy [3], and bridging atom [4] in graphene. In this talk, the role of mediator atoms in two dimensional materials will be introduced in detail and the control of magnetic moment in Fe dopants in graphene [5] will be discussed. If time allows, I will introduce recent results on linear defects in MoS2, graphene partial dislocations [6], and Si atoms at the edge of graphene [7]

References

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Figures

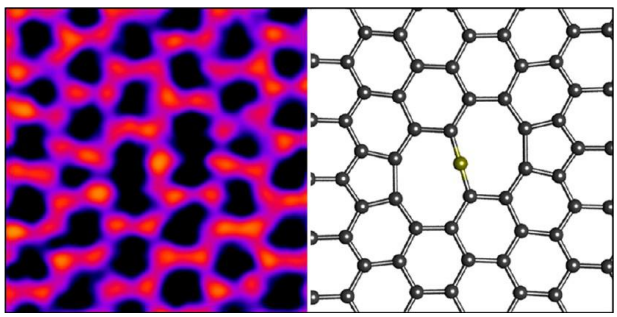

Figure 1 AC-TEM image of a bridging atom stabilized trivacancy and the structural model

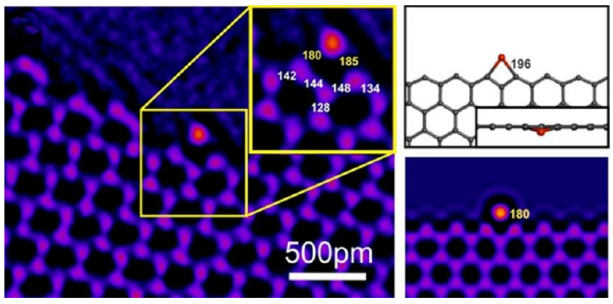

Figure2 Si-C bond at the edge of graphene