Defects and Dopants in Two Dimensional Materials: Collaborative Study of AC-TEM and Simulations

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A Defects and Dopants in two dimensional materials have become a subject of intensive investigation. In order to observe and control the defects and dopants, 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 sometimes difficult to observe the detail of the formation process even within the state-of-the-art microscopy methods because the dynamics of defect and dopant structures 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 AC-TEM, the tight-binding molecular dynamics simulation and density functional theory (DFT) calculation. From the cooperative research, we studied the hydrogen-free graphene edges [2], the stability and dynamics of tetravacancy [3], bridging atom [4], and metal dopants [5] in graphene. In this talk, graphene partial dislocations [6],and the linear defects [7] and metal dopants [8] in MoS2 will be discussed and the role of mediator atoms in two dimensional materials will be introduced.

References

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Figures

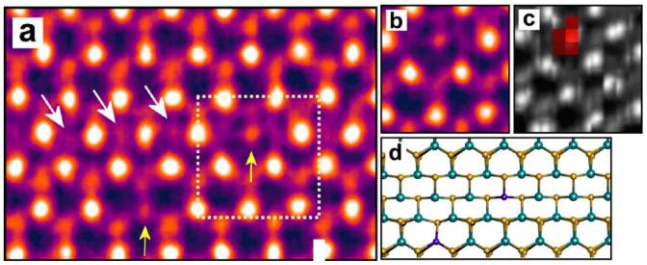

Figure 1: Inclusion of Cr substitutions in S vacancy line defects. (a) ADF-STEM image of a 2SVL defect, with both a Cr@Mo in the bulk lattice and one imbedded in the line center (yellow arrows). White arrows indicate single S atoms within the SVL. (b) ADF-STEM image and (c) EELS map of the boxed region in (a). (d) Atomic model of (a)

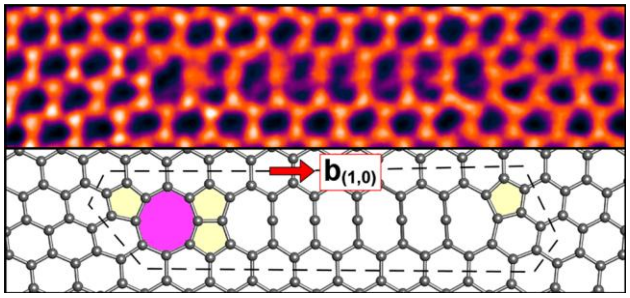

Figure 2: Partial Dislocations in Graphene. AC-TEM imagesand the structural model