

## 点缺陷石墨烯的电导

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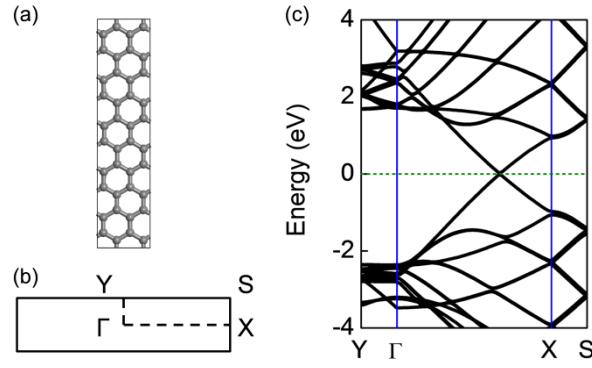
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## Electrical Conductance of Graphene with Point Defects

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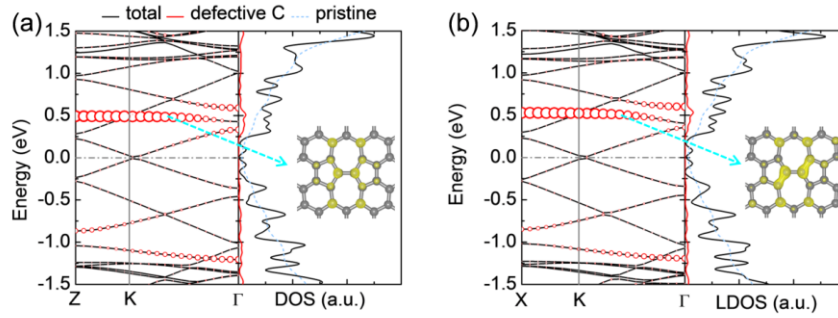
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**Fig. S1** (a) Atomic structure of graphene lead; (b) first Brillouin zone of the graphene lead; (c) band structure of graphene lead with a  $50 \times 5 \times 1$   $k$ -point mesh.

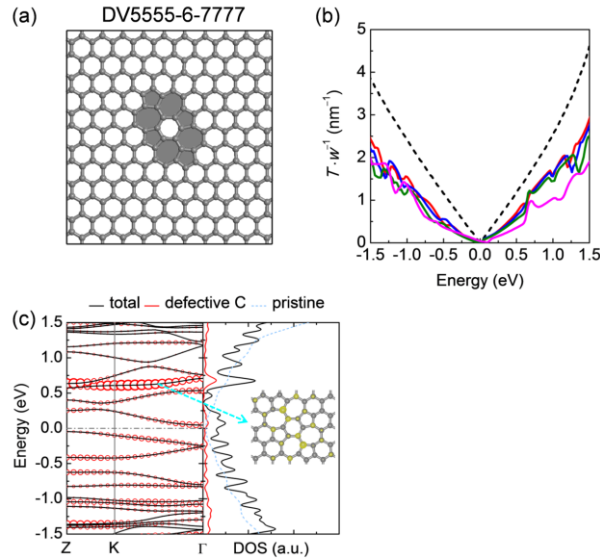
The Fermi energy is shifted to zero.



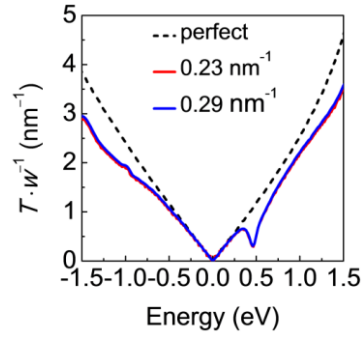
**Fig. S2** Band structures and density of states (DOS) for SW defect at concentration of  $0.39 \text{ nm}^{-1}$  calculated by the SCF convergence criteria of (a)  $10^{-4}$  and (b)  $10^{-6}$  eV.

The red circles in the left panel show the bands from C atoms in the defect region, and the radius of the circles is proportional to the weight. In the right panel, the black solid line shows the total DOS of defected graphene monolayer, the red solid line shows the DOS from C atoms in the defect region, and the light blue dashed line shows the DOS of perfect graphene.

The insets display the partial charge densities of the localized states indicated by the cyan dashed arrows, with an isosurface value of  $1.5 e^{-}\text{nm}^{-1}$ . The Fermi level is set to zero.

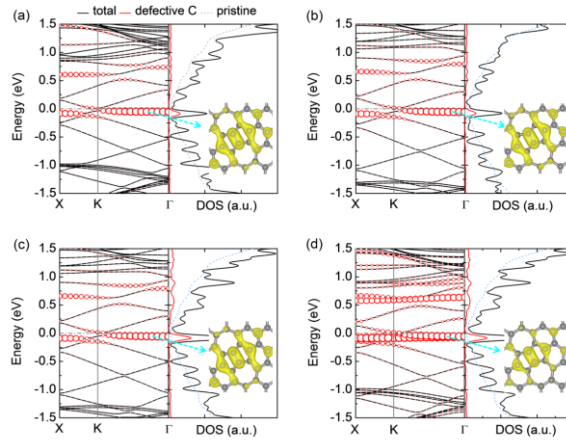


**Fig. S3** (a) Atomic structure of graphene with DV5555-6-7777 defect at concentration of  $0.39 \text{ nm}^{-1}$ . (b) Transmission spectrum per unit width ( $T \cdot w^{-1}$ ) for DV5555-6-7777 at various defect concentrations (colored solid lines). The transmission spectrum of perfect graphene is shown by black dashed line. The Fermi energy is shifted to zero. (c) Band structure (left panel) and density of states (DOS) (right panel) of DV5555-6-7777 at defect concentration of  $0.39 \text{ \AA}^{-1}$ . In the left panel, the red circles show the bands from C atoms in the defect region, and the radius of the circles is proportional to the weight. In the right panel, the black solid line shows the total DOS of defected graphene monolayers, the red solid lines show the DOS from C atoms in the defect region, and the light blue dashed line shows the DOS of perfect graphene. The insets display the partial charge densities of the localized states indicated by the cyan dashed arrows, with an isosurface value of  $1.5 e^{-}\text{nm}^{-1}$ . The Fermi energy is shifted to zero.



**Fig. S4** Transmission spectrum per unit width ( $T \cdot w^{-1}$ ) for SW defect with  $c = 0.23$  and  $0.29 \text{ nm}^{-1}$ .

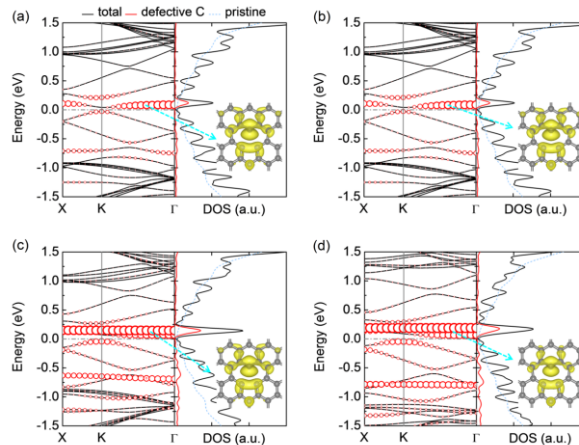
The transmission spectrum of perfect graphene is shown by black dashed line. The Fermi energy is shifted to zero.



**Fig. S5** Band structure (left panels) and density of states (DOS) (right panels) of graphene monolayer with inverse-SW defect at various concentrations: (a)  $0.29 \text{ nm}^{-1}$ , (b)  $0.39 \text{ nm}^{-1}$ , (c)  $0.58 \text{ nm}^{-1}$  and (d)  $0.78 \text{ nm}^{-1}$ .

In the left panels, the red circles show the bands from C atoms in the defect region, and the radius of the circles is proportional to the weight. In the right panels, the black solid line shows the total DOS of defected graphene monolayers, the red solid lines show the DOS from C atoms in the defect region, and the light blue dashed line shows the DOS of perfect graphene. The insets display the partial charge densities of the localized states indicated by the cyan dashed arrows, with an isosurface value of  $1.5 e^{-} \text{ nm}^{-1}$ .

The Fermi energy is shifted to zero.



**Fig. S6** Same as Fig. S5 for graphene with SV5-9 defect.

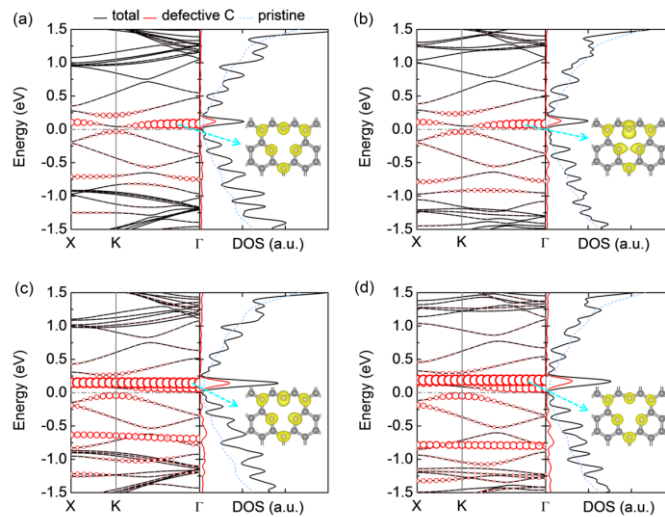


Fig. S7 Same as Fig. S5 for graphene with SV defect.

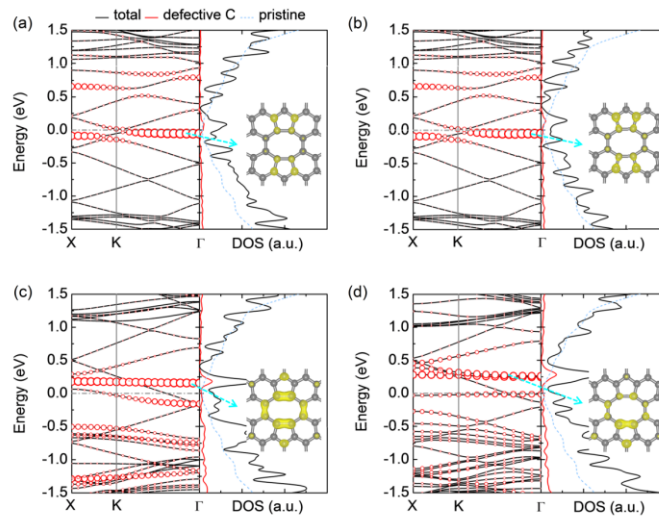


Fig. S8 Same as Fig. S5 for graphene with DV585 defect.

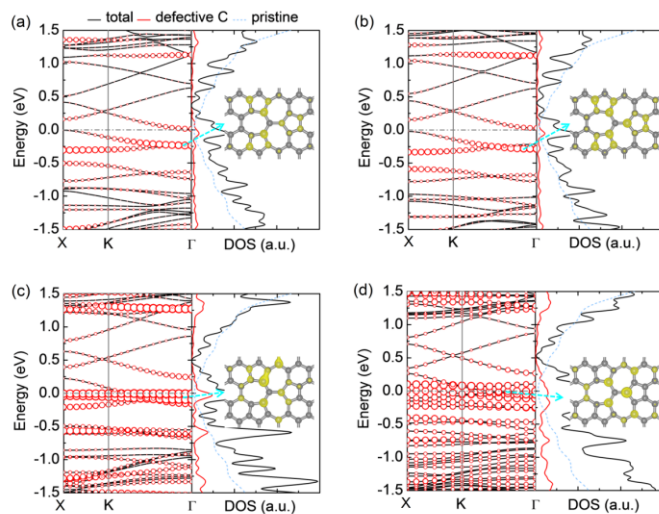


Fig. S9 Same as Fig. S5 for graphene with DV555777 defect.

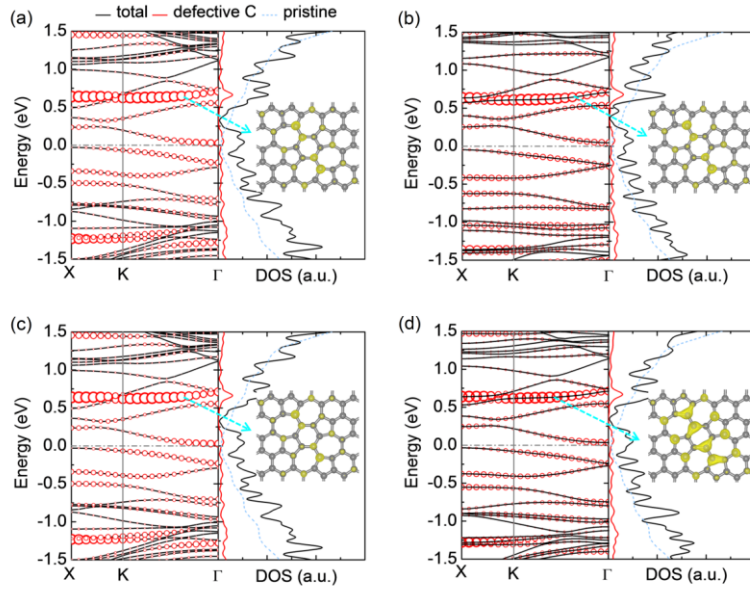


Fig. S10 Same as Fig. S5 for graphene with DV5555-6-7777 defect.

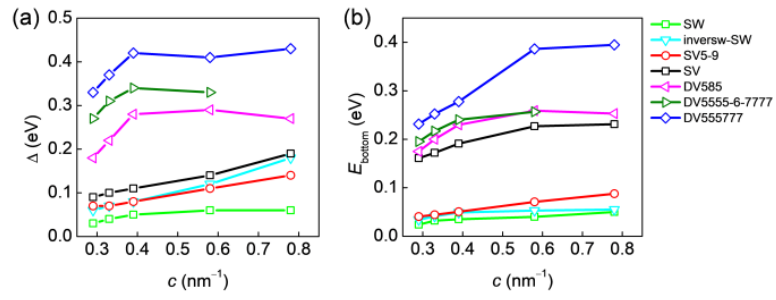


Fig. S11 Energy splitting ( $\Delta$ ) and (b) energy of the band bottom to the Fermi energy ( $E_{\text{bottom}}$ ) as a function of defect concentration ( $c$ ) for various types of point defect.