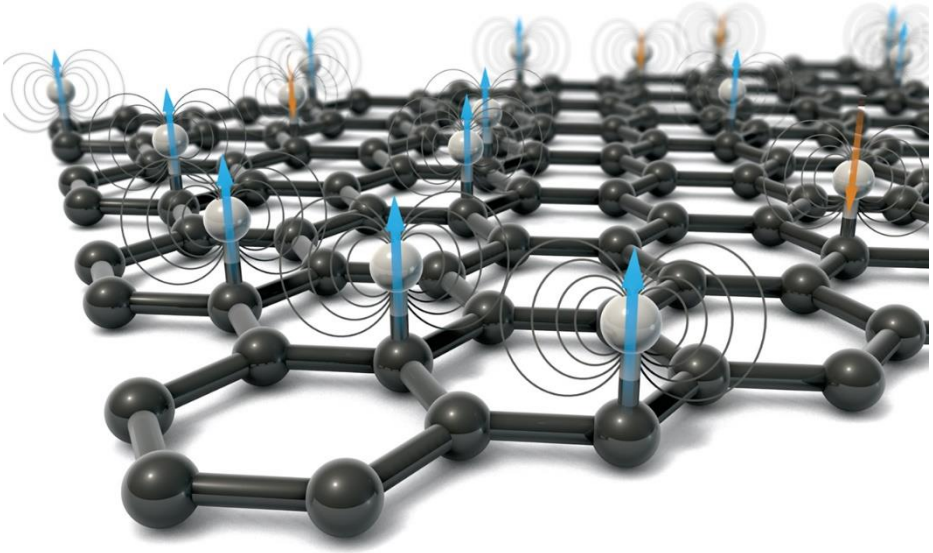
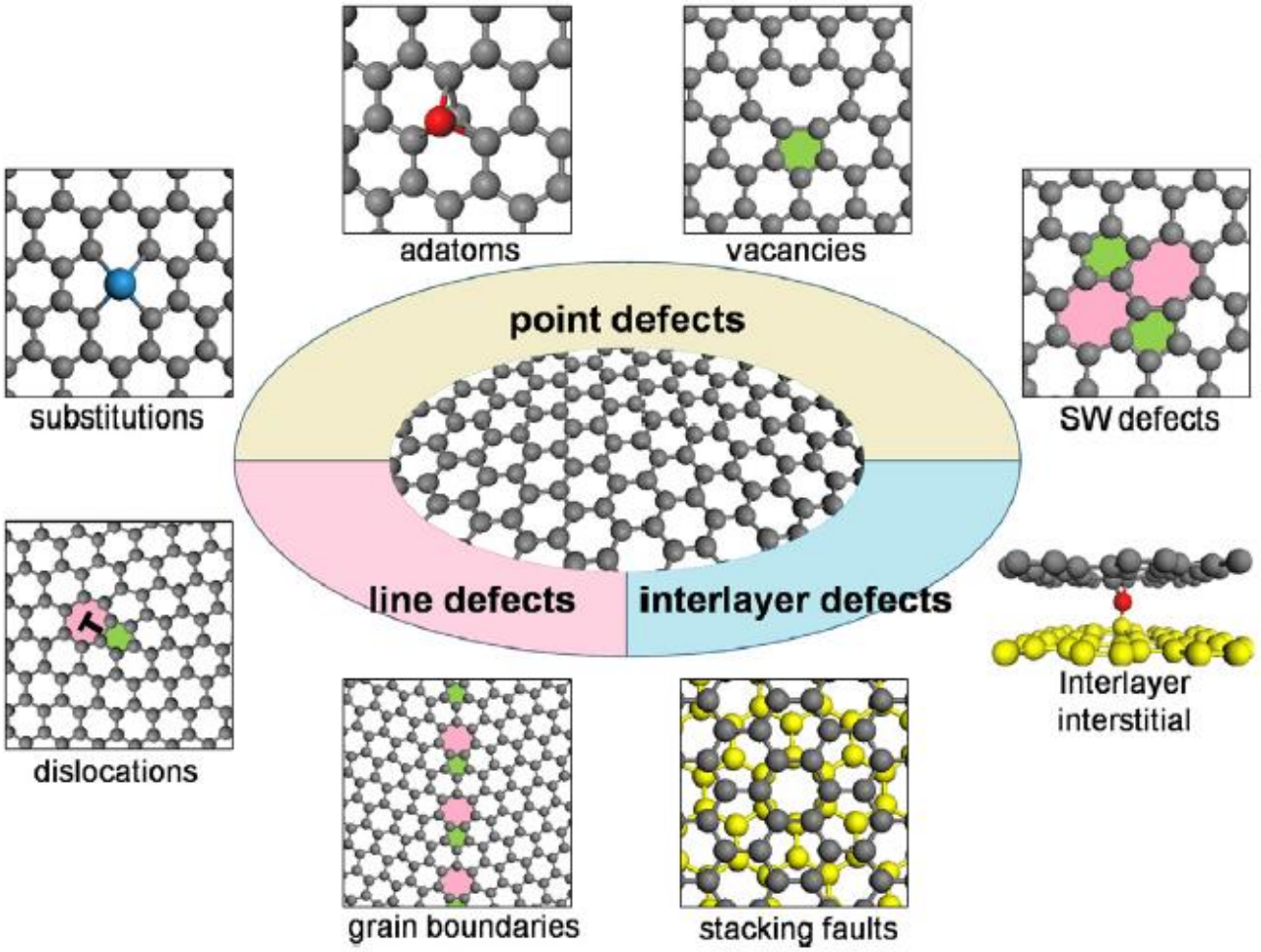
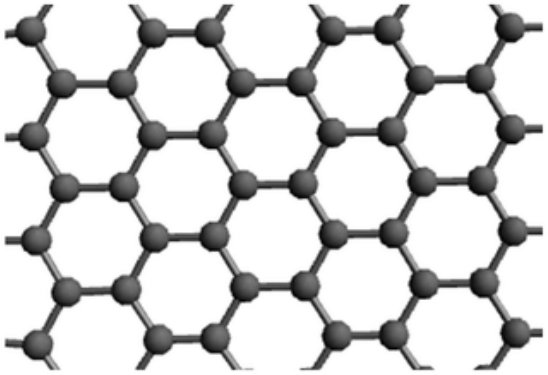
Lattice Defects in Graphene: Types, Generation, Effects and Regulation





Defects in graphene. Similar to the case in macroscopic crystalline materials, structural defects in graphene have different dimensionalities.

Zero-dimensional point defects consist of StoneWales defects, vacancies, adatoms, and substitutions.
One-dimensional line defects emerge in different situations from those in bulk crystals due to the reduced dimensionality. Not only edge dislocations but also grain boundaries are 1D lines along which atoms are arranged anomalously.
Interstitial between the layers can bridge the adjacent layers, forming higher dimensional structures.
Stacking fault is another typical defect in few-layer graphene.



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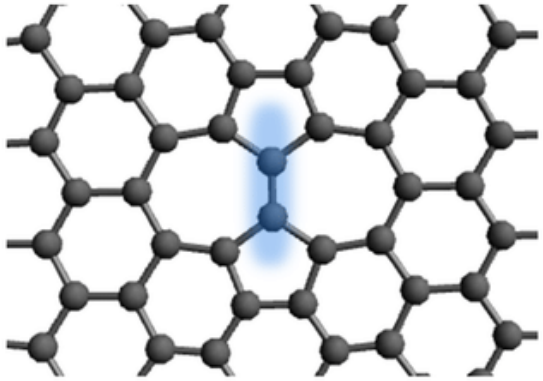
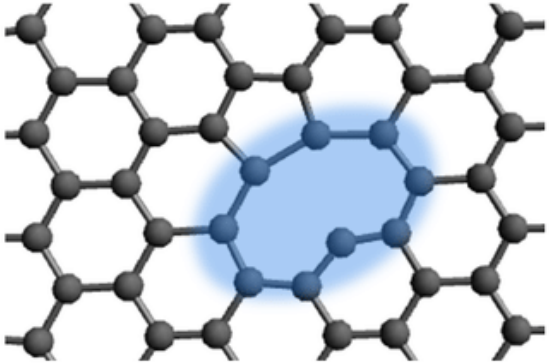
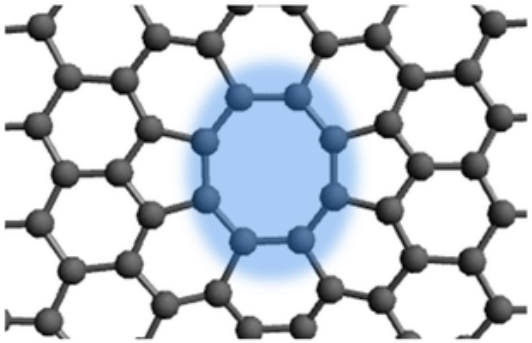


Stone-Wales defect



Single vacancy



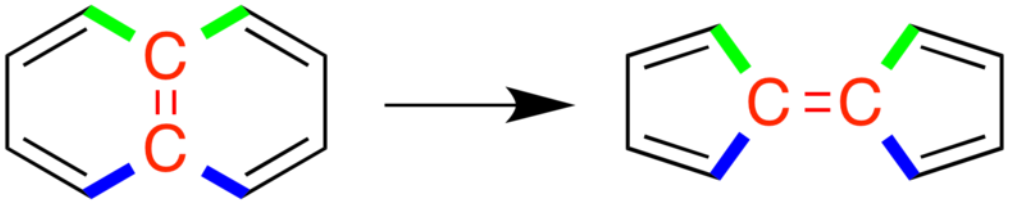
Double vacancy

Principal defects of graphene:
Stone-Wales defect, single vacancy and double vacancy.

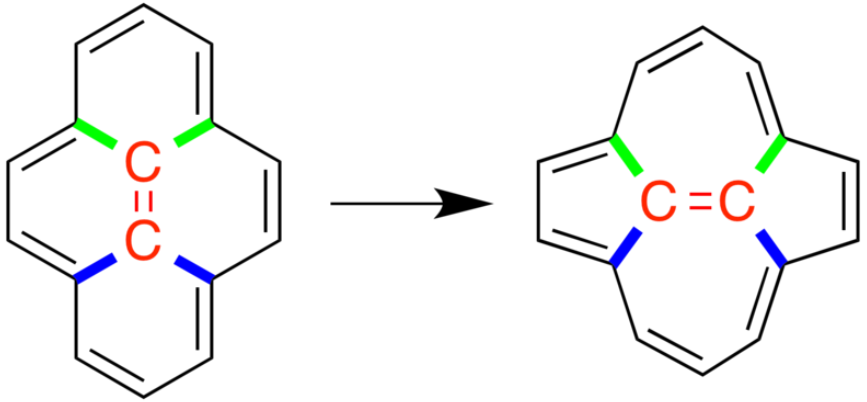
Stone–Wales defect

A Stone–Wales defect is a crystallographic defect that involves the change of connectivity of two π-bonded carbon atoms, leading to their rotation by 90° with respect to the midpoint of their bond.

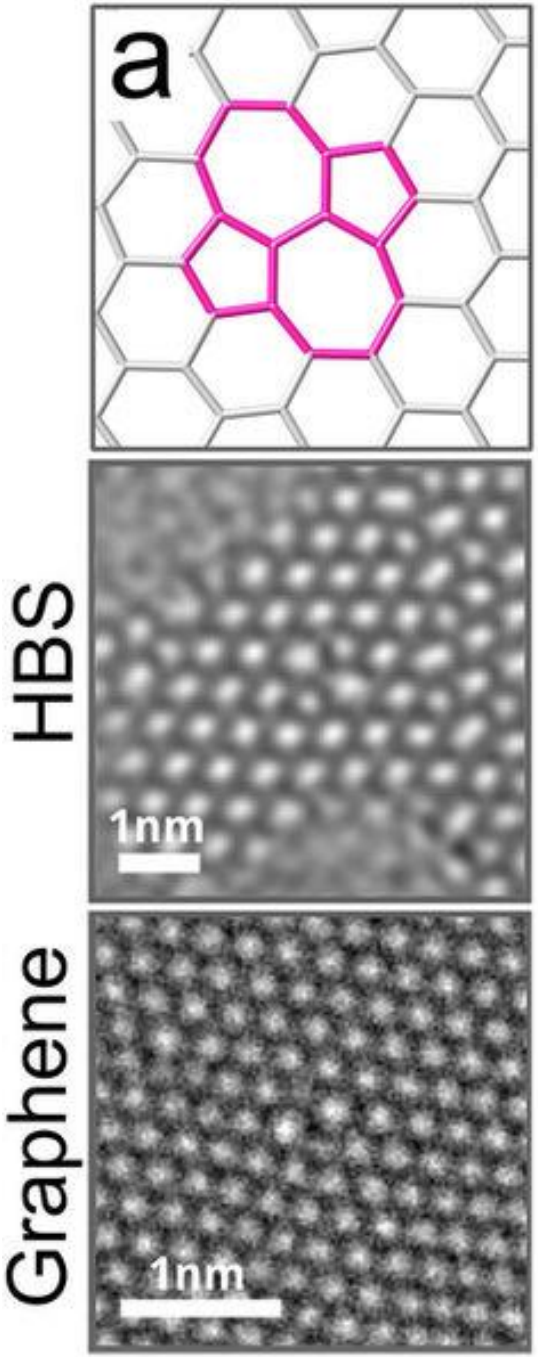
The reaction commonly involves conversion between a naphthalene-like structure into a fulvalene-like structure, that is, two rings that share an edge vs two separate rings that have vertices bonded to each other.



Skeletal structures for the conversion of naphthalene into fulvalene, highlighting the Stone–Wales defect rearrangement details.



Skeletal structures for the conversion of pyrene by a Stone–Wales defect rearrangement



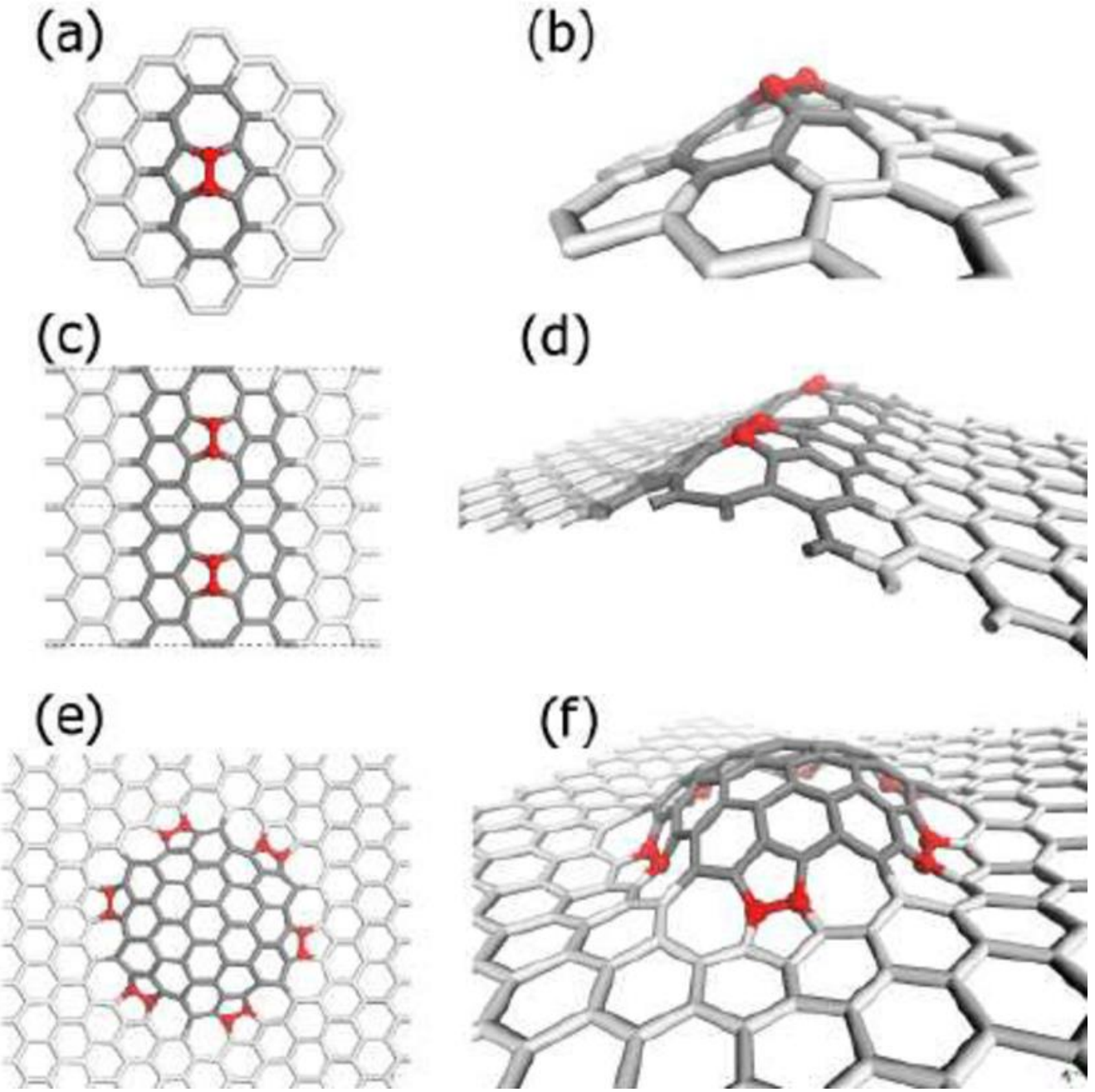
Stone–Wales defect

StoneWales (SW) defects resulting from CC bond rotation without atoms gained or lost are also considered as 0D defects.

Atomic models (top row) and AC-HRTEM images of Stone-Wales defects in HBS and graphene (middle and bottom rows, respectively).

History

The defect is named after Anthony Stone and David J. Wales at the University of Cambridge, who described it in a 1986 paper[4] on the isomerization of fullerenes.


(a)
(b)
(c)
(d)
(e)
(f)

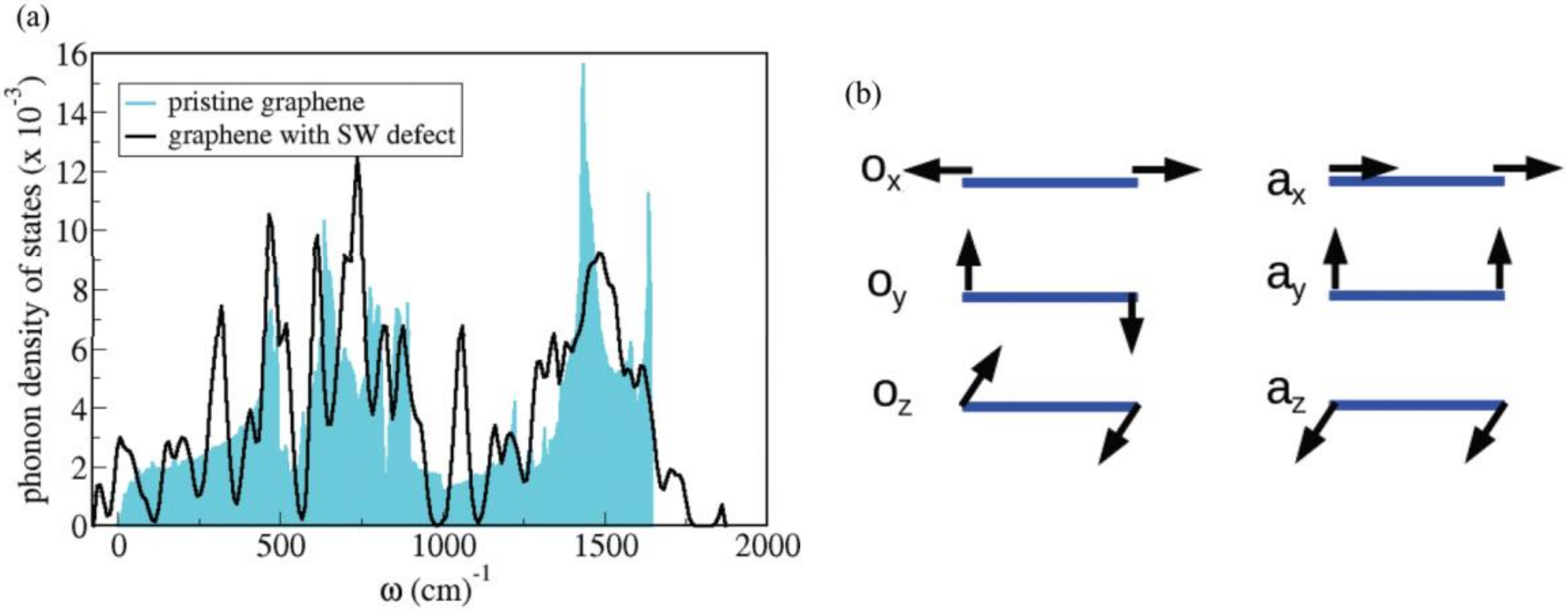


FIG. (Color online) Phonon density of states and eigendisplacements in graphene. (a) Phonon density of states of pristine graphene and graphene with SW defects (for 2.04% concentration of defects). Light blue (gray) and black denote the phonon density of states for pristine graphene and graphene with SW defects, respectively. (b) Eigendisplacements of optical and acoustic modes in graphene.

Nucleation and Growth of Carbon Nanostructures

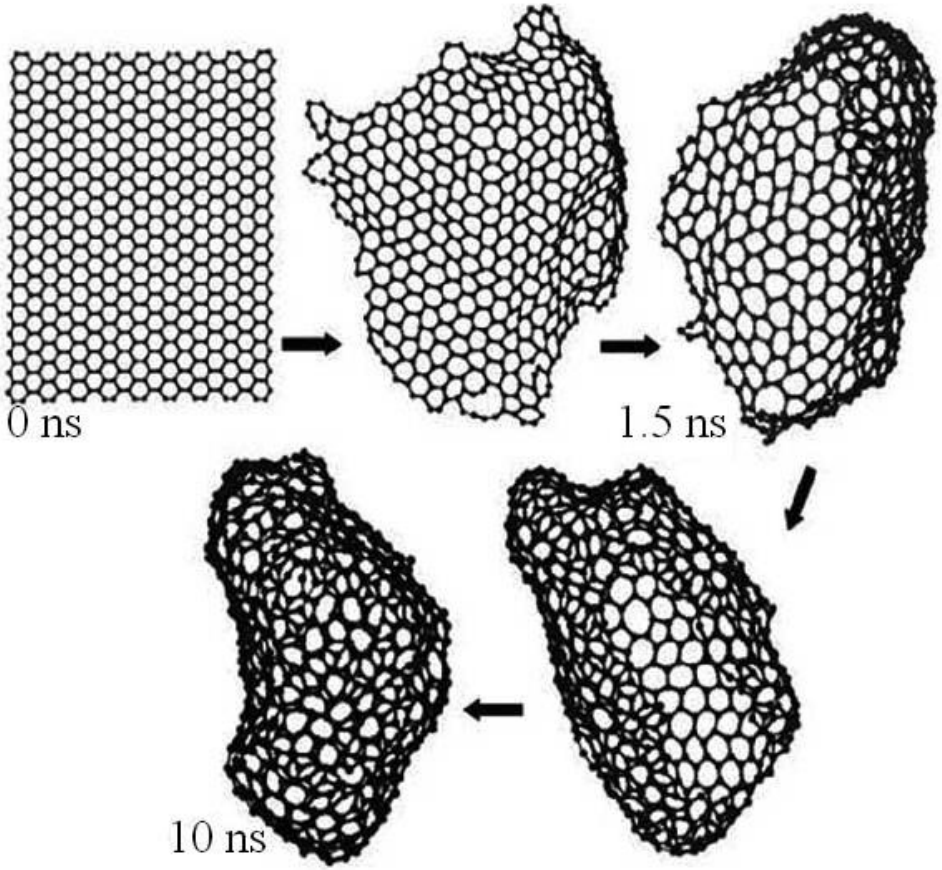


Fig.1. Evolution of a graphite sheet at 3500K.

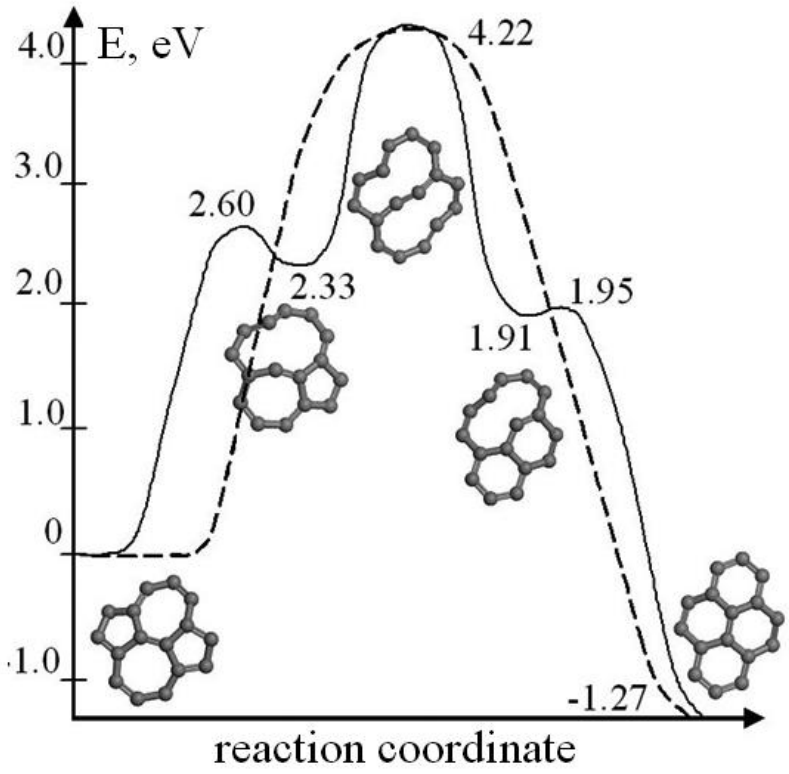
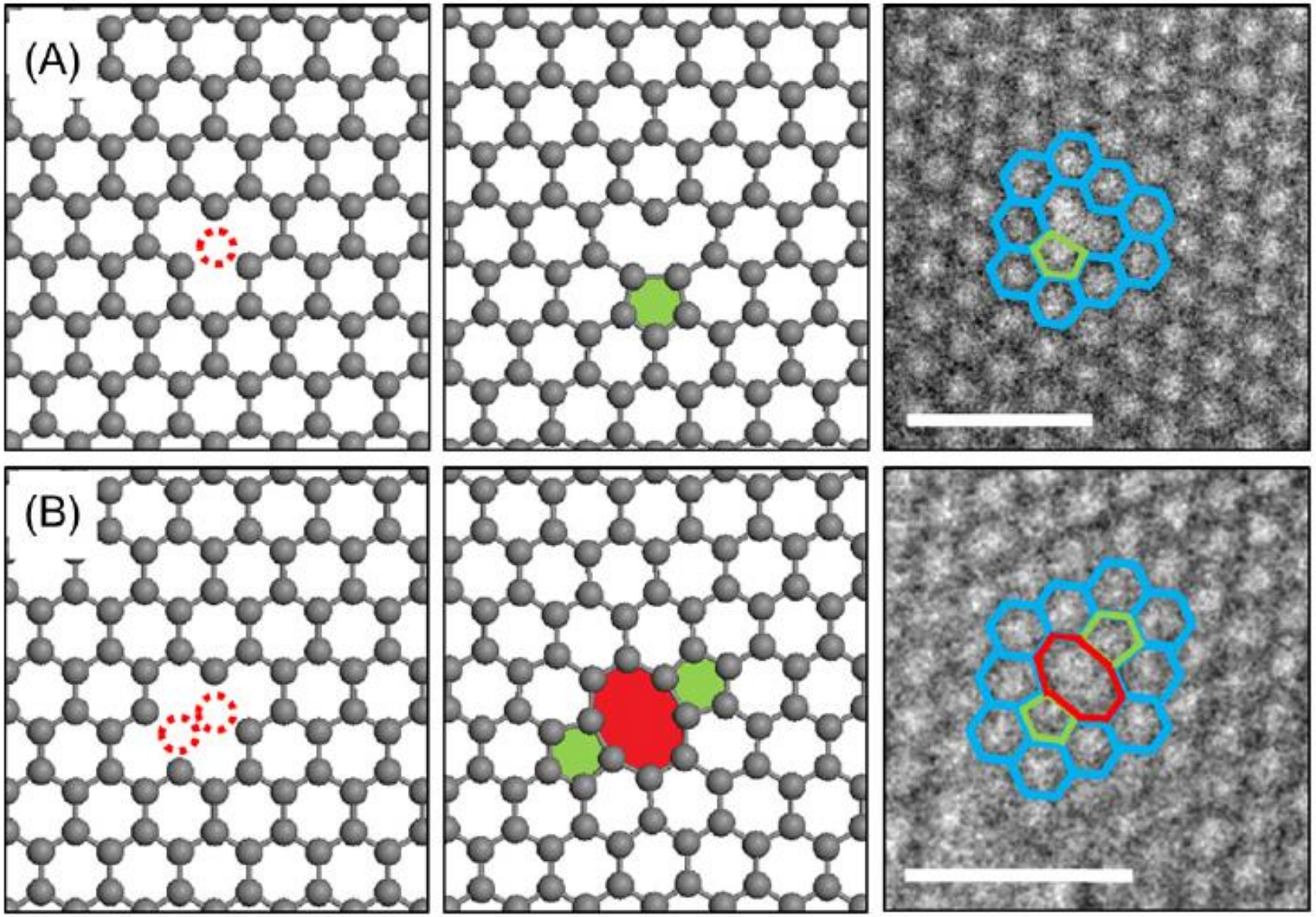


Fig 2. Calculated reaction pathway of t
Stone-Wales rearrangement of defects
the gas phase.

Vacancies in graphene



Vacancies