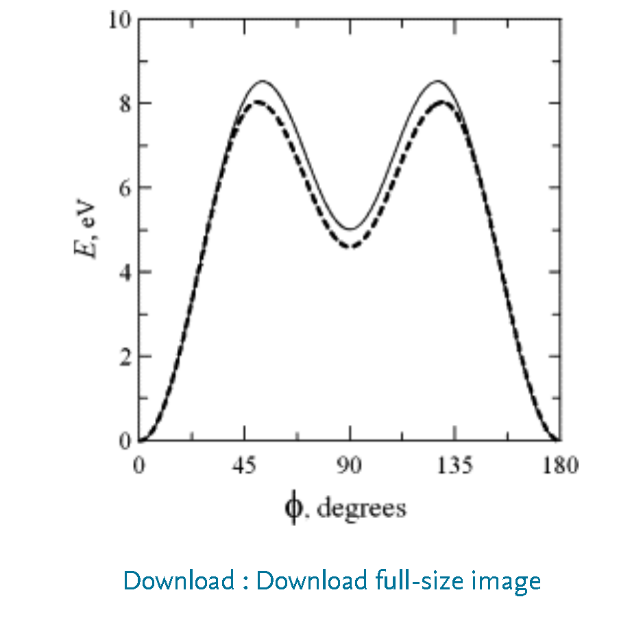
**Out-of-plane path of the Stone–Wales transformation in graphene**

<https://www.sciencedirect.com/science/article/pii/S0375960115003394#fg0020>

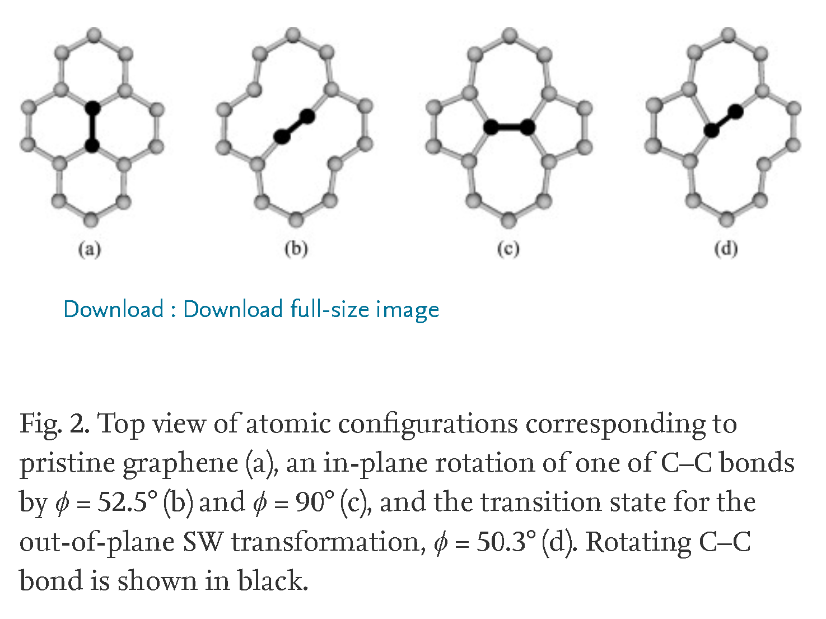
Supercell size: 160 atoms

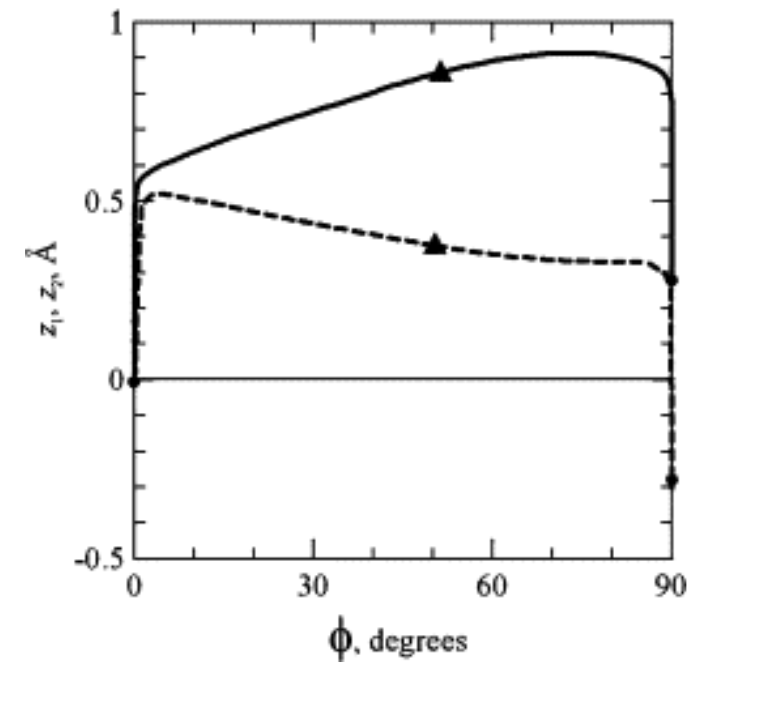
Method: nonorthogonal tight-binding model

For FSWT

 ϕm=52.5°

Uf=E(ϕ=ϕm)−E(ϕ=0)=8.52eV

Fig. 1. Energy E of a 160-atom graphene supercell versus the angle ϕ of C–C bond rotation. Solid curve relates to in-plane bond rotation resulting in a flat SW defect (the rotated atoms do not displace in the vertical direction). Dashed curve corresponds to the non-planar SW transformation bringing about the formation of a buckled sinelike SW defect (both atoms of the rotated bond move out of plane, and the angle ϕ quantifies the rotation of the C–C bond projection on a graphene plane).

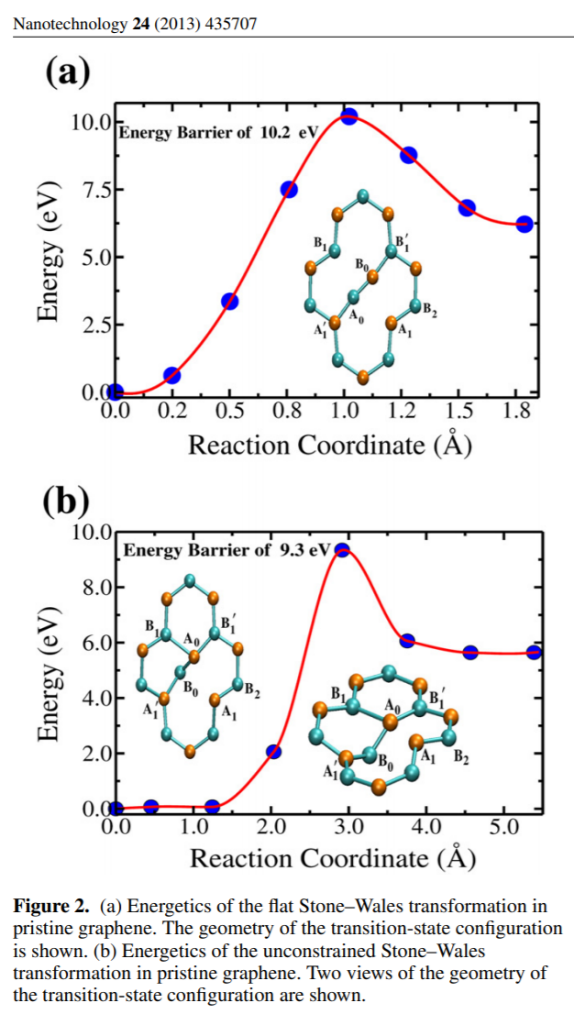
For out of plane SWT: energy peaks at ϕm=50.3°, energy barriers U to formation and annealing of the sinelike SW defect are, respectively, Uf=8.03eV and Ua=3.43eV, each being by ΔU=0.49eV lower than for the in-plane path.

**Lubrication of Stone–Wales transformations in graphene by hydrogen and hydroxyl functional groups**

<https://iopscience-iop-org.ezproxy.lib.calpoly.edu/article/10.1088/0957-4484/24/43/435707/pdf>

Method: projector augmented wave method within DFT (Formation energies of defects, chemisorption energies of functional groups, and activation barriers of SWTs)

Reaction paths, TSCs, and the corresponding energy barriers 1ETSC were determined using the climbing-image nudged-elastic-band method

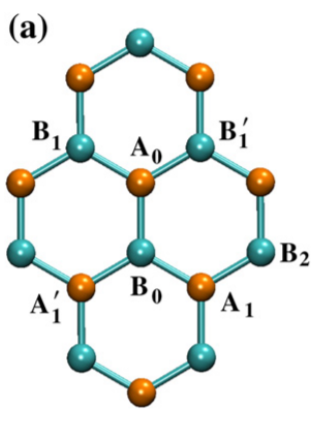
The exchange–correlation functional was treated by the generalized gradient approximation [35] with the parameterization scheme of Perdew, Burke, and Ernzerhof. A plane-wave-basis set with a cutoff energy of 400 eV was used for computation of the energetics of the SWT transformations, and a 500 eV cutoff was used for computation of the formation energies and chemisorption energies of the stable (or metastable) configurations.

Energy Barriers: EFTSC = 10.2 eV EUTSC = 9.3 eV

Discusses rearrangement of other atoms in the FSWT:

A1–B1 distance is substantially larger than in the pristine lattice.

The A0–B0 bond length is 1.29 A and the A ˚ 0–B0 1 and A0 1 –B0 bonds are shortened to 1.36 A, from 1.42 ˚ A in pristine graphene.

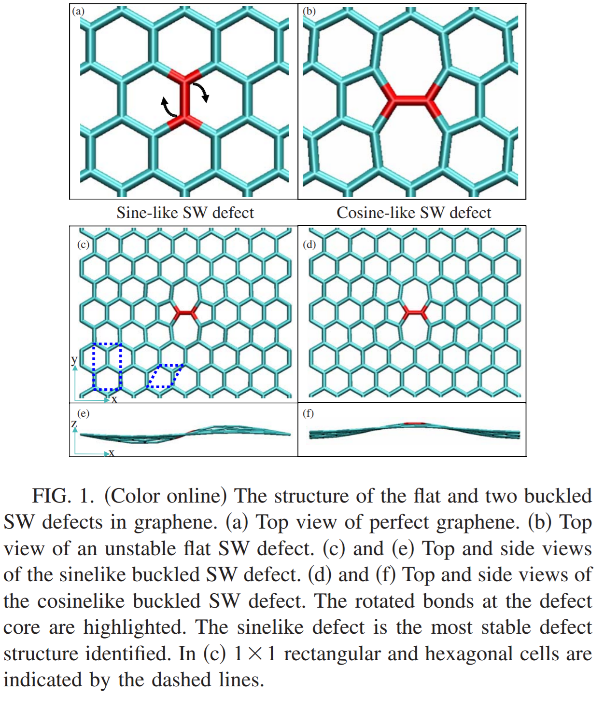
Discussion of transition state in USWT:

In the UTSC, while the C atoms at the A0 and B’1 sites remain in the graphene plane, that on the B0 site shifts ‘down’ by −0.95 A, being accompanied by the A’1 and B1 atoms, which shift off-plane by −0.52 A and ˚ −0.15 A, respectively. ˚ The larger upwards shift are experienced by the A1 site (0.47 A) and one of its neighbors (0.40 ˚ A) in the perimeter ˚ of the SW defect.

**Stone-Wales defects in graphene and other planar sp2-bonded materials**

Method: The DFT calculations reported herein have been performed with the plane-wave code CPMD. 20 Troullier-Martins norm-conserving pseudopotentials21 are employed with an energy cutoff of 100 Ry

<https://journals-aps-org.ezproxy.lib.calpoly.edu/prb/pdf/10.1103/PhysRevB.80.033407>

Not much discussion of transition state in this one, besides:

This sinelike structure is a true minimum with no imaginary frequencies, whereas the cosinelike structure is a transition state with one imaginary frequency.

**Stone−Wales Transformation in Double-Walled Carbon Nanotubes and the Role of Inner Tube**

Method: B3LYP/6-31G

The optimized geometry of transition states as obtained from the B3LYP/6-31G\* method was taken as the initial geometry for the Car−Parrinello molecular dynamics (CPMD) simulations.

<https://pubs.acs.org/doi/10.1021/jp208329y>

**Scratching the Surface of Buckminsterfullerene:  The Barriers for Stone−Wales Transformation through Symmetric and Asymmetric Transition States**

General-gradient approximation (PBE) and hybrid Hartree−Fock density functional theories (B3LYP) in conjunction with basis sets of up to polarized triple-ζ quality have been applied to study the Stone−Wales transformation of buckminsterfullerene (BF)

<https://pubs.acs.org/doi/10.1021/ja0288744>

**Kinetics of Topological Stone−Wales Defect Formation in SingleWalled Carbon Nanotubes**

DFT coupled with climbing-image nudge elastic band method.

The DFT calculations are carried out within the projector augmented wave potential implemented in the Vienna ab initio simulation package.

<https://pubs.acs.org/doi/10.1021/acs.jpcc.5b11682>