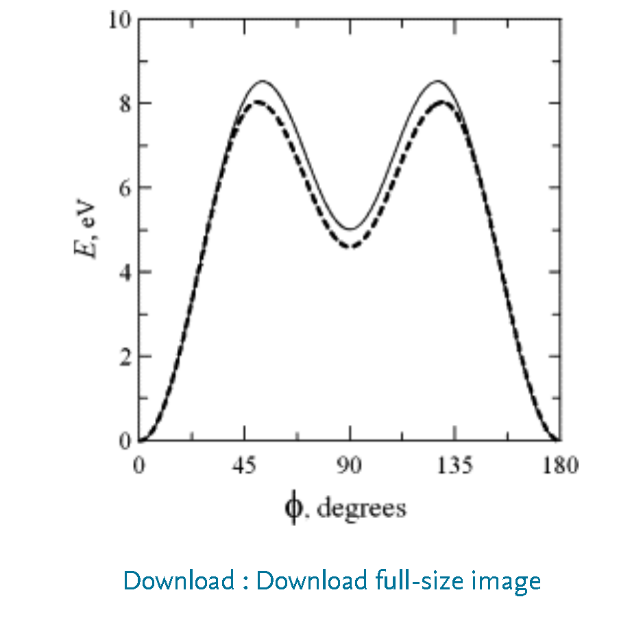
**Out-of-plane path of the Stone–Wales transformation in graphene**

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

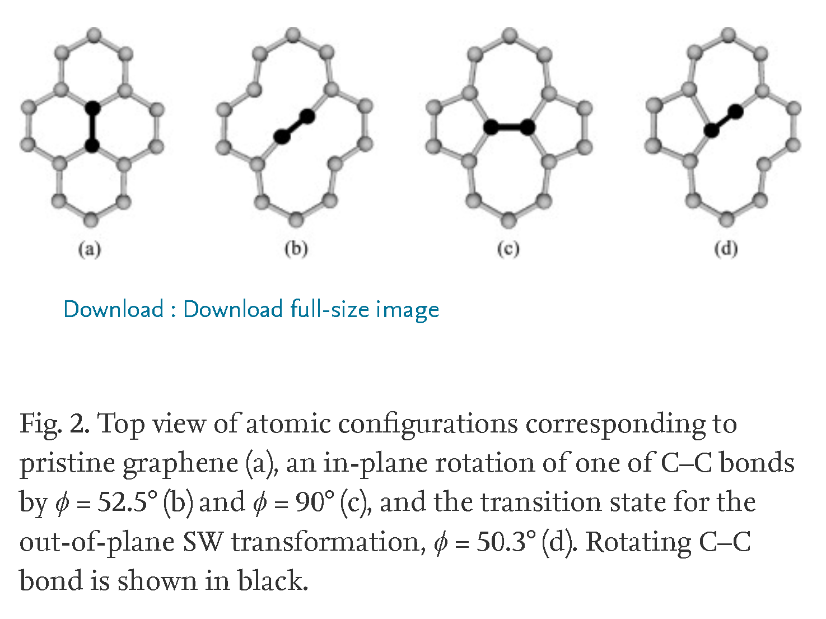
Supercell size: 160 atoms

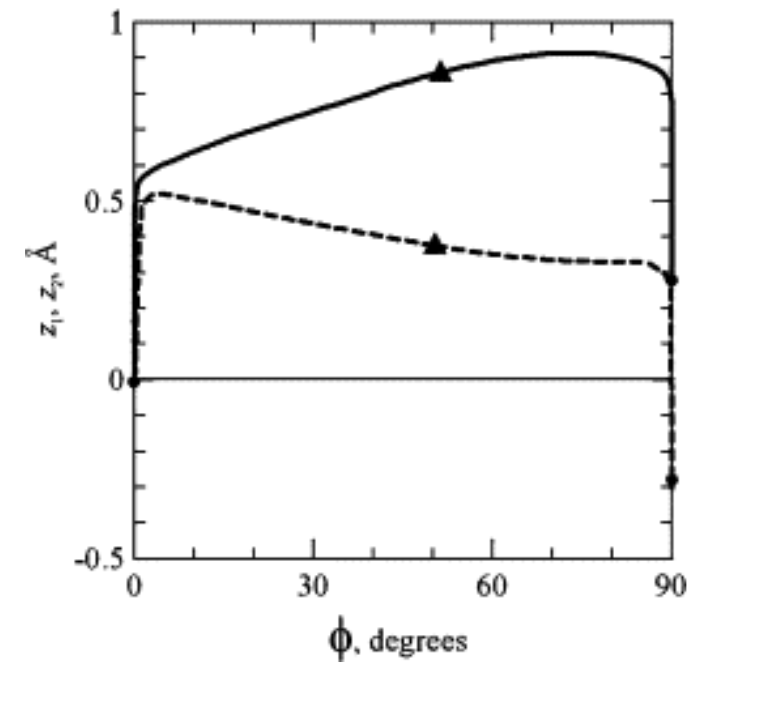
Method: nonorthogonal tight-binding model

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).

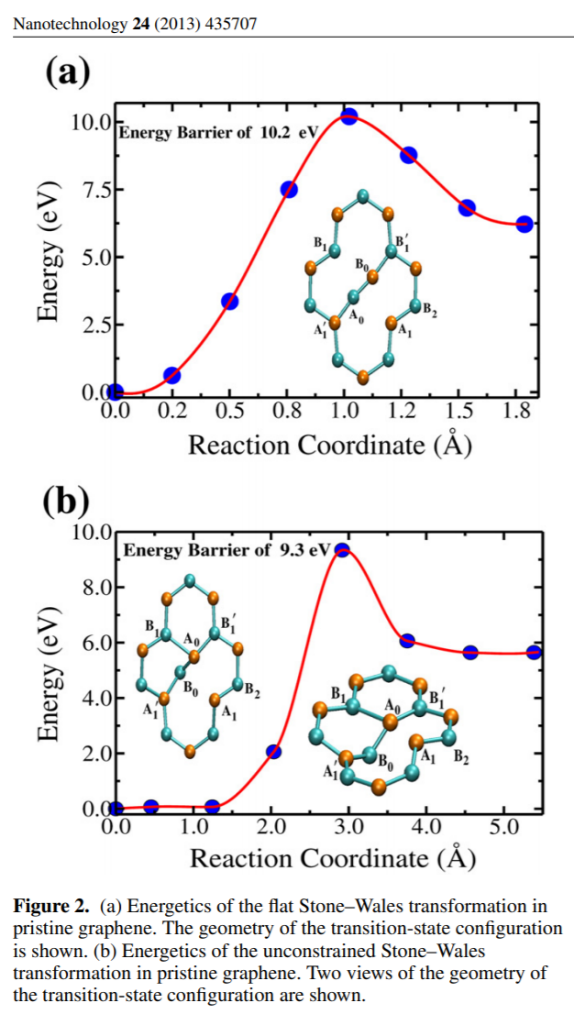
For out of plane SWT: energy peaks at ϕm=50.3°, energy barriers U to formation and annealing of the sinelike SW defect are, respectively, Uf=8.03eV and Ua=3.43eV, each being by ΔU=0.49eV lower than for the in-plane path.

**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

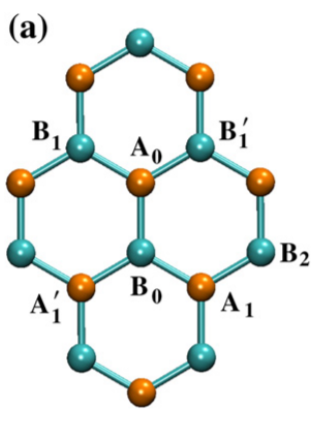
The exchange–correlation functional was treated by the generalized gradient approximation [35] with the parameterization scheme of Perdew, Burke, and Ernzerhof. A plane-wave-basis set with a cutoff energy of 400 eV was used for computation of the energetics of the SWT transformations, and a 500 eV cutoff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

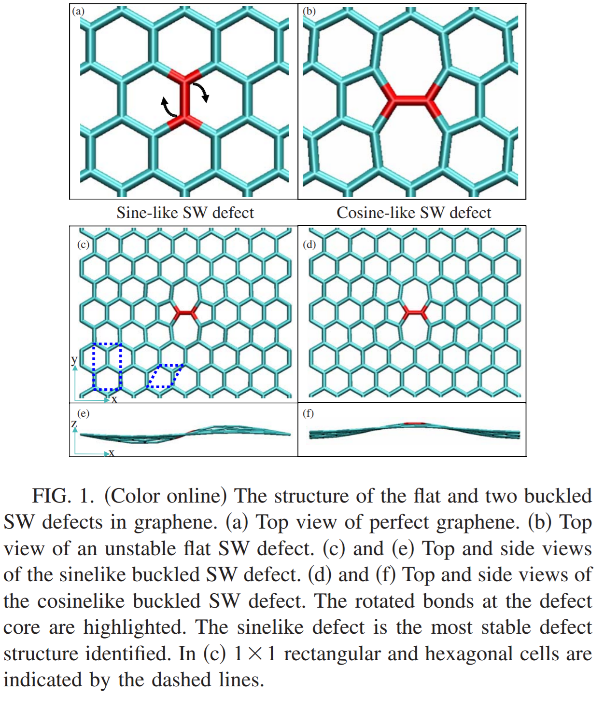
Discussion of transition state in USWT:

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.

**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>

**Adsorption properties of hydrogen on (10,0) single-walled carbon nanotube through density functional theory**

<https://www.sciencedirect.com/science/article/pii/S0008622304002842>

The DMol3 package [[16]](https://www.sciencedirect.com/science/article/pii/S0008622304002842" \l "BIB16) from [Molecular Simulation](https://www.sciencedirect.com/topics/materials-science/molecular-simulation), Inc. which was installed in a 16-CPU (Intel Pentium IV 2.4 GHz) cluster computer was used for all the calculations in this DFT study of the hydrogen-CNT system. The exchange-correlation energy in the [generalized gradient approximation](https://www.sciencedirect.com/topics/engineering/generalized-gradient-approximation) (GGA) was parameterized by Perdew and Wang's scheme [[17]](https://www.sciencedirect.com/science/article/pii/S0008622304002842" \l "BIB17). All the electron Kohn–Sham wave functions were expanded in a local atomic orbital basis. All the orbitals including core electrons were taken into account throughout the calculations. The unrestricted Hartree–Fock (UHF) method with a double-numerical basis set [[18]](https://www.sciencedirect.com/science/article/pii/S0008622304002842" \l "BIB18) was also used to describe the polarization functions (DNP), equivalent to split-valence double-zeta plus polarization basis set quality, which is accepted as the standard basis set in quantum chemistry.

When the length was smaller than that of C100H20, the physisorption [energy](https://www.sciencedirect.com/topics/engineering/energy-engineering) was affected by the edge atom of the tube; therefore we chose the C100H20 tube.

**Density Functional Theory (DFT) Study of O2, N2 Adsorptions on H-Capped (5, 0) Single–Walled Carbon Nanotube (CNT)**

<https://www.hindawi.com/journals/jchem/2012/819490/>

Geometry optimizations were performed using 6-311G\* basis set with B3LYP functional

**Adsorption performance of Rh decorated SWCNT upon SF6 decomposed components based on DFT method**

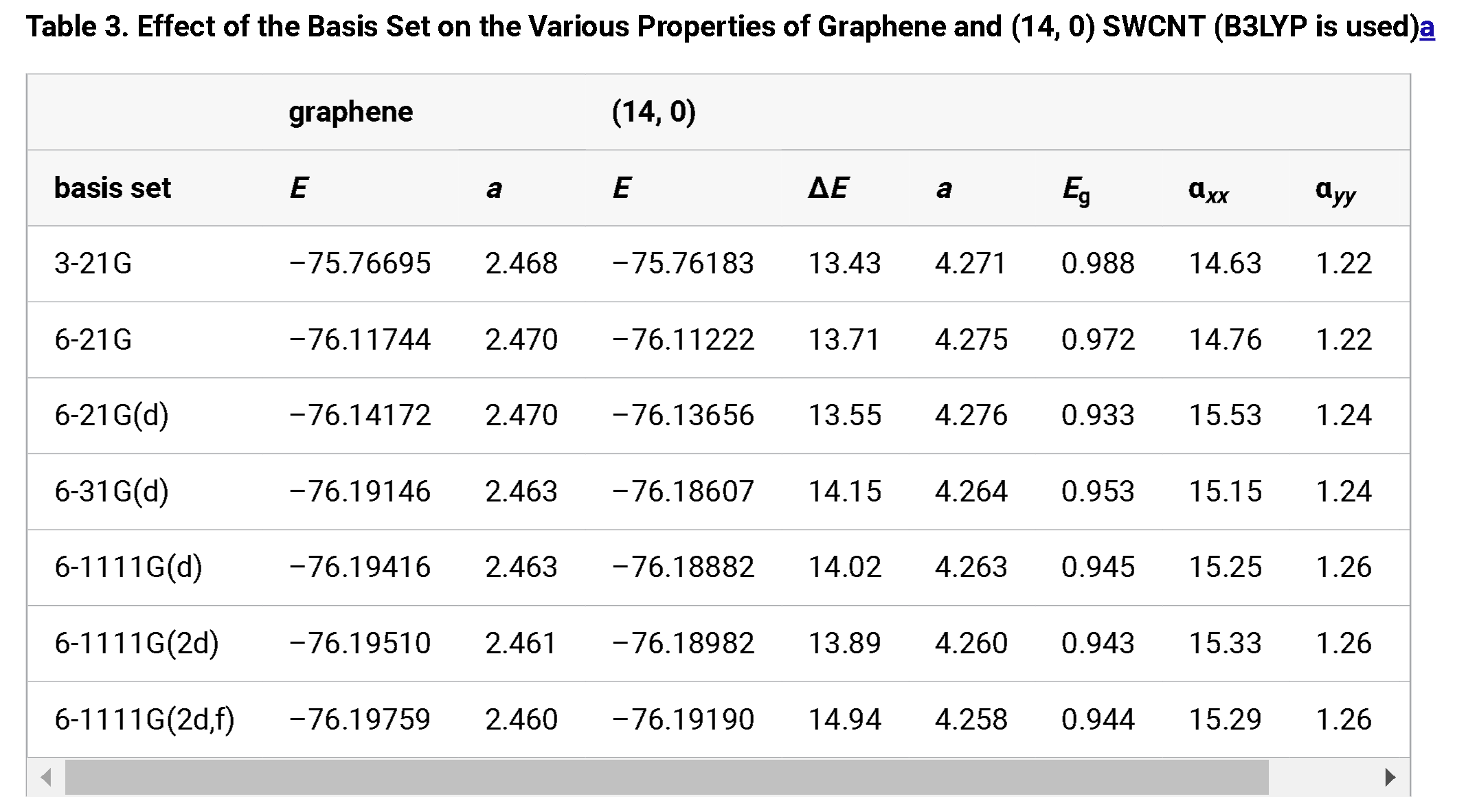
<https://www.sciencedirect.com/science/article/pii/S0169433217314502>

The double numerical plus polarization (DNP) basis sets were applied in the [density functional theory](https://www.sciencedirect.com/topics/chemistry/density-functional-theory) (DFT) calculations based on the Dmol3 package [[12]](https://www.sciencedirect.com/science/article/pii/S0169433217314502" \l "bib0060). The [generalized-gradient approximation](https://www.sciencedirect.com/topics/chemistry/generalized-gradient-approximation) (GGA) with the Perdew-Burke-Emzerhof (PBE) and Spin-unrestricted DFT [[13]](https://www.sciencedirect.com/science/article/pii/S0169433217314502" \l "bib0065) is employed to obtain all the results reported below. In order to avoid the interaction between adjacent cells, a [single wall carbon nanotube](https://www.sciencedirect.com/topics/chemistry/single-walled-nanotube) (SWCNT) with periodic boundary condition 20 Å × 20 Å × 8.5 Å was defined [[14]](https://www.sciencedirect.com/science/article/pii/S0169433217314502" \l "bib0070). The core treatment was set as DFT Semi-core Pseudopots to manage the interaction between the nucleus and valence electron, whereas the [Brillouin zone](https://www.sciencedirect.com/topics/chemistry/brillouin-zone) k-point sampling was performed in 1 × 1 × 2 Monkhorst-Pack mesh [[15]](https://www.sciencedirect.com/science/article/pii/S0169433217314502" \l "bib0075), [[16]](https://www.sciencedirect.com/science/article/pii/S0169433217314502" \l "bib0080) that presents good approximation for (8, 0) SWCNTs.

**Properties of Carbon Nanotubes: An ab Initio Study Using Large Gaussian Basis Sets and Various DFT Functionals**

<https://pubs.acs.org/doi/full/10.1021/jp110704x>

Calculations were performed with the CRYSTAL09 periodic ab initio code,[(42)](javascript:void(0);) which exploits the helical symmetry for automatic generation of the nanotube structure starting from a two-dimensional layer, for mono- and bielectronic integral calculation and for Fock matrix diagonalization.[(9, 43)](javascript:void(0);)

All-electron Gaussian type basis sets of increasing size, from 3-21G[(49)](javascript:void(0);) to 6–1111G(2d,f), were used (3-21G, 6-21G, and 6–21G(d) from ref [49](javascript:void(0);), 6-31G(d) and 6-1111G from ref [50](javascript:void(0);), 6-1111G(d), 6-1111G(2d), and 6-1111G(2d,f) obtained by adding one d, αd1 = 0.8325 bohr–2, two d, αd1 = 0.6786, and αd2 = 1.02 bohr–2, and a further f, αf = 0.8 bohr–2, orbitals to 6-1111G[(50)](javascript:void(0);)). Twelve DFT functionals, corresponding to three levels of approximation of the exchange-correlation contribution (LDA: SVWN[(51, 52)](javascript:void(0);) and SPWLSD;[(51, 53)](javascript:void(0);) GGA: PBE,[(54)](javascript:void(0);) PW91,[(55)](javascript:void(0);) PBEsol,[(6)](javascript:void(0);) SOGGA-[(8)](javascript:void(0);) and WC-[(7)](javascript:void(0);)PBE; hybrids: B1WC,[(56)](javascript:void(0);) WC1LYP,[(29)](javascript:void(0);) B3PW,[(57)](javascript:void(0);) B3LY,P[(58, 59)](javascript:void(0);) and PBE0[(60)](javascript:void(0);)), were tested.

E: electronic energy [Eh per two C atoms]; ΔE: energy difference with respect to graphene [kJ/mol per two C atoms]; a: lattice parameter [Å]; Eg: band gap [eV

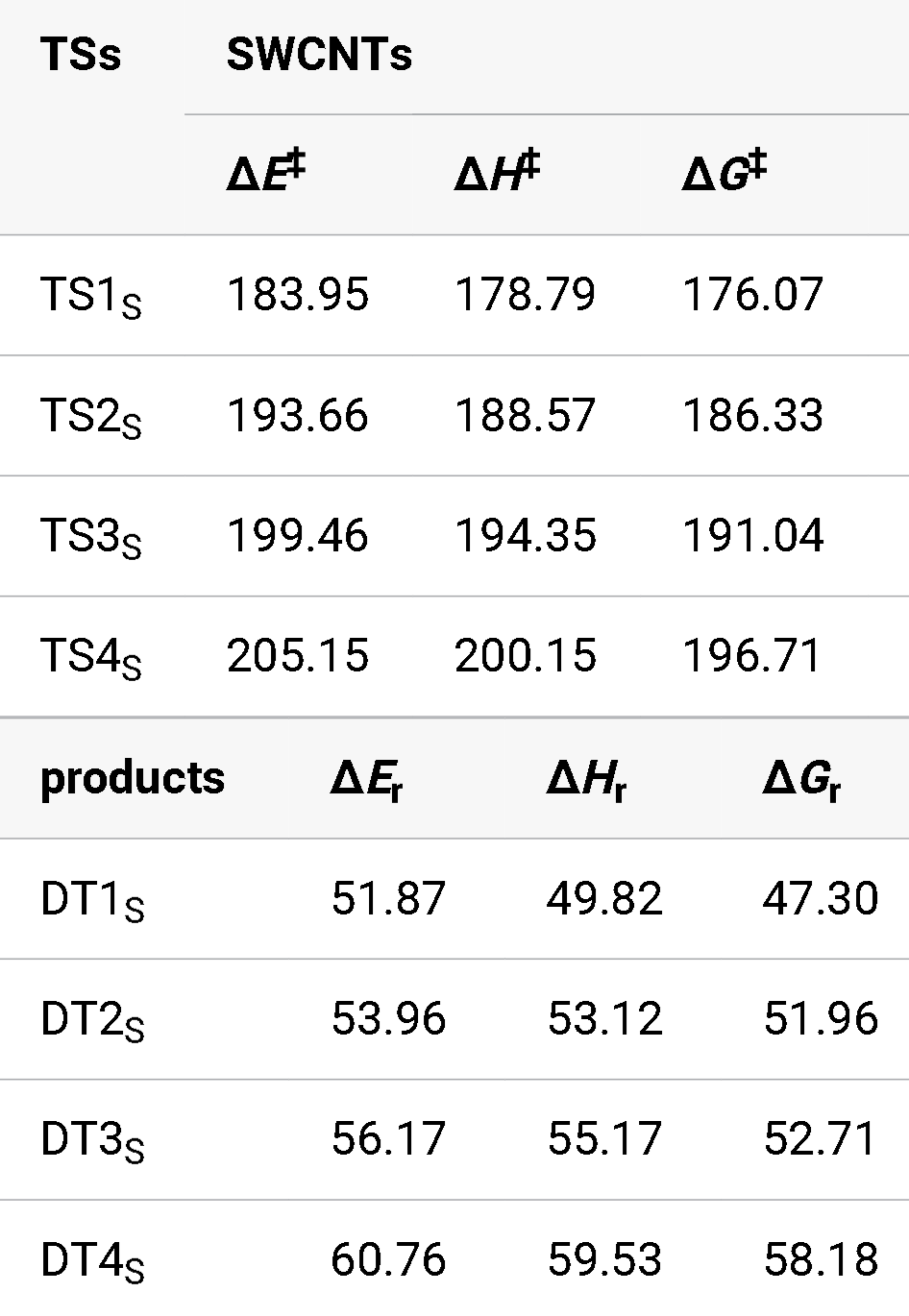
Obviously, a better description of the core electrons has a strong influence on the total electronic energy (E): when passing from 3-21G to 6-21G, E decreases by 350 mEh for graphene.

PBE and PW91 tend to overestimate the geometrical parameters, whereas LDA underestimates them. The recently proposed GGA functionals (PBEsol, WC-PBE, and SOGGA) improve the performance with respect to PBE and PW91, providing structural results comparable to those obtained with hybrid functionals. The five hybrid functionals give, in general, a better description of the structure, WC1LYP, B3PW, and PBE0 providing the least deviation from experiments.

**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>

7.97 eV

(8,0) 2.249 eV

(10,0)

(12,0)

(14,0)