Table of Features

Benyamin Motevalli, Baichuan Sun, and Amanda S. Barnard*

Data61 CSIRO, Docklands, Victoria 3008, Australia

E-mail: amanda.barnard@csiro.au

Provided in this document are details of the simulation method used to generate the data, and a table of features.

To generate this set of graphene oxide nanoflakes we have used density functional tight-binding method with self-consistent charges (SCC-DFTB) as implemented in the DFTB+ code[1] to perform the individual calculations,[2,3] since the tight-binding methodology has been shown to be ideal for studying the electronic properties of graphene[4]. The SCC-DFTB is an approximate quantum chemical approach where the Kohn-Sham density functional is expanded to second order around a reference electron density. The reference density is obtained from self-consistent density functional calculations of weakly confined neutral atoms within the generalized gradient approximation (GGA). The confinement potential is optimised to anticipate the charge density and effective potential in molecules and solids. A minimal valence basis set is used to account explicitly for the two-centre tight-binding matrix elements within the DFT level. The double counting terms in the Coulomb and exchange-correlation potential, as well as the intra-nuclear repulsion are replaced by a universal short-range repulsive potential. Finally, the self-consistency is included at the level of Mulliken charges, which are an intrinsic part of the Hamiltonian.[2]

The sp^2 hybridized graphene leads to a full-filled σ band and a half-filled π band with one electron in a p orbital. The half-filled bands in transition elements play an important role in the physics of strongly correlated systems since, due to their strong tight-binding character,

large Coulomb energies (leading to strong collective effects and magnetism), and insulating behavior due to correlation gaps or Mottness[5]. Commonly used DFT exchange-correlation functionals that are continuum approximations, such as conventional generalized gradient approximation (GGA) functionals, do not exhibit an integer discontinuity. Thus DFT is not the first selection for the accurate calculation of the electronic structures in the systems with strong correlation. Tight-binding scheme including up to third-nearest neighbors describes the electronic structures accurately consistent with the results from the first principles DFT, with a specific basis set[6], and has proven to be an effective method for studying various properties including electronic structures in graphene.[4] Detailed explicit comparison of DFTB with DFT have been published elsewhere.[7,8]

The each configuration was optimised without constraints until forces on each atom are less than 10^{-4} a.u. ≈ 5 meV Å^{-1}. In all the calculations, the PBC set of parameters[9] is used to describe the contributions from diatomic interactions of hydrogen, oxygen, and carbon. In our case the Fermi level is smeared by 300 K, which leads to the electronic temperature of 1 meV, and we only considered non-magnetic states. This method has been extensively applied to study the energetic and electronic properties of a range of carbon nanostructures and found to be reliable,[10–35] and provide realistic results with respect to other higher order methods and experiment[36–39] under different conditions.[40–43] Data sets generated in this way have been used previously for machine learning.[8,45–47]

A comprehensive structural analysis was performed to extract 830 structural features. These features are grouped into four main categories: thermodynamic (1 feature), structural (19 features), chemical (20 features), and statistical (790 features). The thermodynamic feature is the probability of observation, which was obtained using a Boltzmann distribution *via* the enthalpy of formation from the DFTB calculations. The 19 structural features characterize different geometrical aspects of the flake such as its average diameter, minimum and maximum dimensions, total area of flake, the anisotropy in the flake, and the zigzag and armchair edge ratios. Also, attributes characterizing defects and out of plane distortions

are included in this group. The 20 chemical features include the number and distribution of atomic and chemical species on each nanoflake (counts and concentration of each species, where concentration is counts normalized by total number of atoms) to provide useful overall information about each structure. Of the 790 statistical features, 16 characterize the atomic coordination of C, H and O; 268 characterize the ring statistics; 91 describes bond lengths between different species; 132 describe bond angles; 268 describe oxygen density distributions; 2 define particle and mass density; and 13 describe the distance distributions between different oxygen groups. The 281 features characterizing the oxygen distribution capture the differences between nanoflakes with similar graphene (primary) structures and oxygen concentrations, but different patterning of oxygen groups on the surface. For this purpose the following Gaussian probability (density) distribution function (PDF) is used:

$$\rho(x, y, z) = \sum_{i=1}^{n_s} e^{-\alpha(r_i - r_{\text{ref}})^2} \tag{1}$$

where r_{ref} is the reference location in space to evaluate the species-dependent probability distribution, r_i is the distance of i^{th} species of type s from the reference location, and α is a smoothing parameter. Here, α is set such that the Gaussian function would fade at a distance $\sim$4 Å(which is higher than van der Waals distance between the species on GO). This PDF can be used to define a local density at any point in space and for any type of species. However, these local densities are not normalized, which presents problems for nanoflakes of finite sizes. Lattice sites around the edges and corners of a nanoflake will have a different local environment than those in the interior; fewer carbons providing fewer opportunities for functionalization. To resolve this the local density of carbon atoms can be used to normalize each density distribution using:

$$\rho^{\text{norm}}(x, y, z) = \frac{\sum_{i=1}^{n_s} e^{-\alpha(r_i - r_{\text{ref}})^2}}{\rho_C(x, y, z)} \tag{2}$$

where ρ_C is the local density of carbon atoms at a reference location (x, y, z). The density

functions in equations 1 and 2 can provide local densities of carbon and oxygen atoms as well as ether and hydroxyl groups. The density functions are sampled at the location of each carbon atom, then different statistics such as mean value, standard deviation, skewness, and kurtosis are calculated in order to characterize the distribution. Based on these criteria a set of additional features are extracted, taking the list to 501. It should be noted that many of these features are empty, but are included for completeness, so that others may decide how to perform the feature elimination on a case by case basis.

There are also included two energetic target property labels.

Table of Features

Column	Description
file_name	the name of the XYZ file of of each graphene oxide configuration provided with this document
STRUCTURAL FEATURES	
C	the total number of C atom in the graphene oxide configuration
H	the total number of H atom in the graphene oxide configuration
O	the total number of O atom in the graphene oxide configuration
atom_number_total	the total number of C+H+O atom in the graphene oxide configuration
C_concentration	the fraction of C atoms in the graphene oxide configuration
H_concentration	the fraction of H atoms in the graphene oxide configuration
O_concentration	the fraction of O atoms in the graphene oxide configuration
defects_count	the number of C atoms involved in defect sites on the relaxed graphene oxide configuration
defects_concentration	the fraction of C atoms involved in the defect sites on the relaxed graphene oxide configuration
max_oop	the maximum out of plane distance of C atom on the relaxed graphene oxide configuration
mae_oop	the mean absolute out of plane distance of C atom on the relaxed graphene oxide configuration
std_oop	the STD of out of plane distance of C atom on the relaxed graphene oxide configuration
rmse_oop	the root mean squared out of plane distance of C atom on the relaxed graphene oxide configuration
residual_oop	the total out of plane distance of all C atom on the relaxed graphene oxide configuration
ether_count	the total number of ether adsorbed on the relaxed graphene oxide configuration
hydroxyl_count	the total number of hydroxyl adsorbed on the relaxed graphene oxide configuration
carboxyl_count	the total number of carboxyl adsorbed on the relaxed graphene oxide configuration
all_agent_group_count	the total number of ALL agents adsorbed on the relaxed graphene oxide configuration
ether_concentration	the fraction of ether adsorbed on the relaxed graphene oxide configuration
hydroxyl_concentration	the fraction of hydroxyl adsorbed on the relaxed graphene oxide configuration
carboxyl_concentration	the fraction of carboxyl adsorbed on the relaxed graphene oxide configuration
def_local_ether_count	the number of ether adsorbed on the defected site of the relaxed graphene oxide configuration
def_local_hydroxyl_count	the number of hydroxyl adsorbed on the defected site of the relaxed graphene oxide configuration
def_local_carboxyl_count	the number of carboxyl adsorbed on the defected site of the relaxed graphene oxide configuration
def_local_other_count	the number of other OH agent adsorbed on the defected site of the relaxed graphene oxide configuration
max_bond_angle	maximum bond angle in the whole structure, in degrees

Continued on next page

Column	Description
max_bond_length	maximum bond length in the whole structure, in nm
mass_density	mass density in g/nm^3
particle_density	number of particles per unit volume (nm^{-3})
C-C:total_number	C-C (C-C) bond length total number
C-C:mean_value	C-C (C-C) bond length mean value
C-C:error	C-C (C-C) bond length statistical error
C-C_sp1-sp1:total_number	C-C (sp1-sp1) bond length total number
C-C_sp1-sp1:mean_value	C-C (sp1-sp1) bond length mean value
C-C_sp1-sp1:error	C-C (sp1-sp1) bond length statistical error
C-C_sp1-sp2:total_number	C-C (sp1-sp2) bond length total number
C-C_sp1-sp2:mean_value	C-C (sp1-sp2) bond length mean value
C-C_sp1-sp2:error	C-C (sp1-sp2) bond length statistical error
C-C_sp1-sp3:total_number	C-C (sp1-sp3) bond length total number
C-C_sp1-sp3:mean_value	C-C (sp1-sp3) bond length mean value
C-C_sp1-sp3:error	C-C (sp1-sp3) bond length statistical error
C-C_sp1-strained:total_number	C-C (sp1-strained) bond length total number
C-C_sp1-strained:mean_value	C-C (sp1-strained) bond length mean value
C-C_sp1-strained:error	C-C (sp1-strained) bond length statistical error
C-C_sp2-sp2:total_number	C-C (sp2-sp2) bond length total number
C-C_sp2-sp2:mean_value	C-C (sp2-sp2) bond length mean value
C-C_sp2-sp2:error	C-C (sp2-sp2) bond length statistical error
C-C_sp2-sp3:total_number	C-C (sp2-sp3) bond length total number
C-C_sp2-sp3:mean_value	C-C (sp2-sp3) bond length mean value
C-C_sp2-sp3:error	C-C (sp2-sp3) bond length statistical error
C-C_sp2-strained:total_number	C-C (sp2-strained) bond length total number
C-C_sp2-strained:mean_value	C-C (sp2-strained) bond length mean value
C-C_sp2-strained:error	C-C (sp2-strained) bond length statistical error
C-C_sp3-sp3:total_number	C-C (sp3-sp3) bond length total number
C-C_sp3-sp3:mean_value	C-C (sp3-sp3) bond length mean value
C-C_sp3-sp3:error	C-C (sp3-sp3) bond length statistical error
C-C_sp3-strained:total_number	C-C (sp3-strained) bond length total number
C-C_sp3-strained:mean_value	C-C (sp3-strained) bond length mean value
C-C_sp3-strained:error	C-C (sp3-strained) bond length statistical error
C-C_strained-strained:total_number	C-C (strained-strained) bond length total number
C-C_strained-strained:mean_value	C-C (strained-strained) bond length mean value
C-C_strained-strained:error	C-C (strained-strained) bond length statistical error
C-C-C:total_number	C-C-C (C-C-C) bond angle total number
C-C-C:mean_value	C-C-C (C-C-C) bond angle mean value
C-C-C:error	C-C-C (C-C-C) bond angle statistical error
C-C-C_C-sp1-C:total_number	C-C-C (C-sp1-C) bond angle total number
C-C-C_C-sp1-C:mean_value	C-C-C (C-sp1-C) bond angle mean value
C-C-C_C-sp1-C:error	C-C-C (C-sp1-C) bond angle statistical error
C-C-C_C-sp2-C:total_number	C-C-C (C-sp2-C) bond angle total number
C-C-C_C-sp2-C:mean_value	C-C-C (C-sp2-C) bond angle mean value
C-C-C_C-sp2-C:error	C-C-C (C-sp2-C) bond angle statistical error
C-C-C_C-sp3-C:total_number	C-C-C (C-sp3-C) bond angle total number

Continued on next page

Column	Description
C-C-C_C-sp3-C:mean_value	C-C-C (C-sp3-C) bond angle mean value
C-C-C_C-sp3-C:error	C-C-C (C-sp3-C) bond angle statistical error
C-C-C_C-strained-C:total_number	C-C-C (C-strained-C) bond angle total number
C-C-C_C-strained-C:mean_value	C-C-C (C-strained-C) bond angle mean value
C-C-C_C-strained-C:error	C-C-C (C-strained-C) bond angle statistical error
C-C-O:total_number	C-C-O (C-C-O) bond angle total number
C-C-O:mean_value	C-C-O (C-C-O) bond angle mean value
C-C-O:error	C-C-O (C-C-O) bond angle statistical error
C-C-O_C-sp1-O:total_number	C-C-O (C-sp1-O) bond angle total number
C-C-O_C-sp1-O:mean_value	C-C-O (C-sp1-O) bond angle mean value
C-C-O_C-sp1-O:error	C-C-O (C-sp1-O) bond angle statistical error
C-C-O_C-sp2-O:total_number	C-C-O (C-sp2-O) bond angle total number
C-C-O_C-sp2-O:mean_value	C-C-O (C-sp2-O) bond angle mean value
C-C-O_C-sp2-O:error	C-C-O (C-sp2-O) bond angle statistical error
C-C-O_C-sp3-O:total_number	C-C-O (C-sp3-O) bond angle total number
C-C-O_C-sp3-O:mean_value	C-C-O (C-sp3-O) bond angle mean value
C-C-O_C-sp3-O:error	C-C-O (C-sp3-O) bond angle statistical error
C-C-O_C-strained-O:total_number	C-C-O (C-strained-O) bond angle total number
C-C-O_C-strained-O:mean_value	C-C-O (C-strained-O) bond angle mean value
C-C-O_C-strained-O:error	C-C-O (C-strained-O) bond angle statistical error
C-O:total_number	C-O (C-O) bond length total number
C-O:mean_value	C-O (C-O) bond length mean value
C-O:error	C-O (C-O) bond length statistical error
C-O_sp1-sp1:total_number	C-O (sp1-sp1) bond length total number
C-O_sp1-sp1:mean_value	C-O (sp1-sp1) bond length mean value
C-O_sp1-sp1:error	C-O (sp1-sp1) bond length statistical error
C-O_sp1-strained:total_number	C-O (sp1-strained) bond length total number
C-O_sp1-strained:mean_value	C-O (sp1-strained) bond length mean value
C-O_sp1-strained:error	C-O (sp1-strained) bond length statistical error
C-O_sp2-sp1:total_number	C-O (sp2-sp1) bond length total number
C-O_sp2-sp1:mean_value	C-O (sp2-sp1) bond length mean value
C-O_sp2-sp1:error	C-O (sp2-sp1) bond length statistical error
C-O_sp2-strained:total_number	C-O (sp2-strained) bond length total number
C-O_sp2-strained:mean_value	C-O (sp2-strained) bond length mean value
C-O_sp2-strained:error	C-O (sp2-strained) bond length statistical error
C-O_sp3-sp1:total_number	C-O (sp3-sp1) bond length total number
C-O_sp3-sp1:mean_value	C-O (sp3-sp1) bond length mean value
C-O_sp3-sp1:error	C-O (sp3-sp1) bond length statistical error
C-O_sp3-sp2:total_number	C-O (sp3-sp2) bond length total number
C-O_sp3-sp2:mean_value	C-O (sp3-sp2) bond length mean value
C-O_sp3-sp2:error	C-O (sp3-sp2) bond length statistical error
C-O_sp3-strained:total_number	C-O (sp3-strained) bond length total number
C-O_sp3-strained:mean_value	C-O (sp3-strained) bond length mean value
C-O_sp3-strained:error	C-O (sp3-strained) bond length statistical error
C-O_strained-sp1:total_number	C-O (strained-sp1) bond length total number
C-O_strained-sp1:mean_value	C-O (strained-sp1) bond length mean value

Continued on next page

Column	Description
C-O_strained-sp1:error	C-O (strained-sp1) bond length statistical error
C-O_strained-strained:total_number	C-O (strained-strained) bond length total number
C-O_strained-strained:mean_value	C-O (strained-strained) bond length mean value
C-O_strained-strained:error	C-O (strained-strained) bond length statistical error
C-O-C:total_number	C-O-C (C-O-C) bond angle total number
C-O-C:mean_value	C-O-C (C-O-C) bond angle mean value
C-O-C:error	C-O-C (C-O-C) bond angle statistical error
C-O-C_C-sp1-C:total_number	C-O-C (C-sp1-C) bond angle total number
C-O-C_C-sp1-C:mean_value	C-O-C (C-sp1-C) bond angle mean value
C-O-C_C-sp1-C:error	C-O-C (C-sp1-C) bond angle statistical error
C-O-C_C-strained-C:total_number	C-O-C (C-strained-C) bond angle total number
C-O-C_C-strained-C:mean_value	C-O-C (C-strained-C) bond angle mean value
C-O-C_C-strained-C:error	C-O-C (C-strained-C) bond angle statistical error
C-O-H:total_number	C-O-H (C-O-H) bond angle total number
C-O-H:mean_value	C-O-H (C-O-H) bond angle mean value
C-O-H:error	C-O-H (C-O-H) bond angle statistical error
C-O-H_C-sp1-H:total_number	C-O-H (C-sp1-H) bond angle total number
C-O-H_C-sp1-H:mean_value	C-O-H (C-sp1-H) bond angle mean value
C-O-H_C-sp1-H:error	C-O-H (C-sp1-H) bond angle statistical error
C-O-H_C-sp2-H:total_number	C-O-H (C-sp2-H) bond angle total number
C-O-H_C-sp2-H:mean_value	C-O-H (C-sp2-H) bond angle mean value
C-O-H_C-sp2-H:error	C-O-H (C-sp2-H) bond angle statistical error
C-O-H_C-strained-H:total_number	C-O-H (C-strained-H) bond angle total number
C-O-H_C-strained-H:mean_value	C-O-H (C-strained-H) bond angle mean value
C-O-H_C-strained-H:error	C-O-H (C-strained-H) bond angle statistical error
C-O-O:total_number	C-O-O (C-O-O) bond angle total number
C-O-O:mean_value	C-O-O (C-O-O) bond angle mean value
C-O-O:error	C-O-O (C-O-O) bond angle statistical error
C-O-O_C-sp1-O:total_number	C-O-O (C-sp1-O) bond angle total number
C-O-O_C-sp1-O:mean_value	C-O-O (C-sp1-O) bond angle mean value
C-O-O_C-sp1-O:error	C-O-O (C-sp1-O) bond angle statistical error
C-O-O_C-sp2-O:total_number	C-O-O (C-sp2-O) bond angle total number
C-O-O_C-sp2-O:mean_value	C-O-O (C-sp2-O) bond angle mean value
C-O-O_C-sp2-O:error	C-O-O (C-sp2-O) bond angle statistical error
C-O-O_C-strained-O:total_number	C-O-O (C-strained-O) bond angle total number
C-O-O_C-strained-O:mean_value	C-O-O (C-strained-O) bond angle mean value
C-O-O_C-strained-O:error	C-O-O (C-strained-O) bond angle statistical error
O-C-O:total_number	O-C-O (O-C-O) bond angle total number
O-C-O:mean_value	O-C-O (O-C-O) bond angle mean value
O-C-O:error	O-C-O (O-C-O) bond angle statistical error
O-C-O_O-sp2-O:total_number	O-C-O (O-sp2-O) bond angle total number
O-C-O_O-sp2-O:mean_value	O-C-O (O-sp2-O) bond angle mean value
O-C-O_O-sp2-O:error	O-C-O (O-sp2-O) bond angle statistical error

Continued on next page

Column	Description
O-C-O_O-sp3-O:total_number	O-C-O (O-sp3-O) bond angle total number
O-C-O_O-sp3-O:mean_value	O-C-O (O-sp3-O) bond angle mean value
O-C-O_O-sp3-O:error	O-C-O (O-sp3-O) bond angle statistical error
O-H:total_number	O-H (O-H) bond length total number
O-H:mean_value	O-H (O-H) bond length mean value
O-H:error	O-H (O-H) bond length statistical error
O-O:total_number	O-O (O-O) bond length total number
O-O:mean_value	O-O (O-O) bond length mean value
O-O:error	O-O (O-O) bond length statistical error
O-O_sp1-sp1:total_number	O-O (sp1-sp1) bond length total number
O-O_sp1-sp1:mean_value	O-O (sp1-sp1) bond length mean value
O-O_sp1-sp1:error	O-O (sp1-sp1) bond length statistical error
O-O_sp1-sp2:total_number	O-O (sp1-sp2) bond length total number
O-O_sp1-sp2:mean_value	O-O (sp1-sp2) bond length mean value
O-O_sp1-sp2:error	O-O (sp1-sp2) bond length statistical error
O-O_sp1-strained:total_number	O-O (sp1-strained) bond length total number
O-O_sp1-strained:mean_value	O-O (sp1-strained) bond length mean value
O-O_sp1-strained:error	O-O (sp1-strained) bond length statistical error
O-O_sp2-strained:total_number	O-O (sp1-strained) bond length total number
O-O_sp2-strained:mean_value	O-O (sp1-strained) bond length mean value
O-O_sp2-strained:error	O-O (sp1-strained) bond length statistical error
O-O_strained-strained:total_number	O-O (strained-strained) bond length total number
O-O_strained-strained:mean_value	O-O (strained-strained) bond length mean value
O-O_strained-strained:error	O-O (strained-strained) bond length statistical error
O-O-H:total_number	O-O-H (O-O-H) bond angle total number
O-O-H:mean_value	O-O-H (O-O-H) bond angle mean value
O-O-H:error	O-O-H (O-O-H) bond angle statistical error
O-O-H_O-sp1-H:total_number	O-O-H (O-sp1-H) bond angle total number
O-O-H_O-sp1-H:mean_value	O-O-H (O-sp1-H) bond angle mean value
O-O-H_O-sp1-H:error	O-O-H (O-sp1-H) bond angle statistical error
O-O-H_O-sp2-H:total_number	O-O-H (O-sp2-H) bond angle total number
O-O-H_O-sp2-H:mean_value	O-O-H (O-sp2-H) bond angle mean value
O-O-H_O-sp2-H:error	O-O-H (O-sp2-H) bond angle statistical error
O-O-H_O-strained-H:total_number	O-O-H (O-strained-H) bond angle total number
O-O-H_O-strained-H:mean_value	O-O-H (O-strained-H) bond angle mean value
O-O-H_O-strained-H:error	O-O-H (O-strained-H) bond angle statistical error
O-O-O:total_number	O-O-O (O-O-O) bond angle total number
O-O-O:mean_value	O-O-O (O-O-O) bond angle mean value
O-O-O:error	O-O-O (O-O-O) bond angle statistical error
O-O-O_O-sp1-O:total_number	O-O-O (O-sp1-O) bond angle total number
O-O-O_O-sp1-O:mean_value	O-O-O (O-sp1-O) bond angle mean value
O-O-O_O-sp1-O:error	O-O-O (O-sp1-O) bond angle statistical error
C-C_coordination_number	C-C average coordination numbers of first neighbours
C-H_coordination_number	C-H average coordination numbers of first neighbours

Continued on next page

Column	Description
C-O_coordination_number	C-O average coordination numbers of first neighbours
C_atoms_only_1_neighbourtotal	total number of C atoms with only 1 neighbour
C_atoms_with_bond_angles_-<_90_deg._total	total number of C atoms with bond angles deg <90 deg.
C_n10_m1	ring statistics, density of 10 membered rings containing 1 C atoms
C_n10_m10	ring statistics, density of 10 membered rings containing 10 C atoms
C_n10_m2	ring statistics, density of 10 membered rings containing 2 C atoms
C_n10_m3	ring statistics, density of 10 membered rings containing 3 C atoms
C_n10_m4	ring statistics, density of 10 membered rings containing 4 C atoms
C_n10_m5	ring statistics, density of 10 membered rings containing 5 C atoms
C_n10_m6	ring statistics, density of 10 membered rings containing 6 C atoms
C_n10_m7	ring statistics, density of 10 membered rings containing 7 C atoms
C_n10_m8	ring statistics, density of 10 membered rings containing 8 C atoms
C_n10_m9	ring statistics, density of 10 membered rings containing 9 C atoms
C_n11_m1	ring statistics, density of 11 membered rings containing 1 C atoms
C_n11_m10	ring statistics, density of 11 membered rings containing 10 C atoms
C_n11_m11	ring statistics, density of 11 membered rings containing 11 C atoms
C_n11_m2	ring statistics, density of 11 membered rings containing 2 C atoms
C_n11_m3	ring statistics, density of 11 membered rings containing 3 C atoms
C_n11_m4	ring statistics, density of 11 membered rings containing 4 C atoms
C_n11_m5	ring statistics, density of 11 membered rings containing 5 C atoms
C_n11_m6	ring statistics, density of 11 membered rings containing 6 C atoms
C_n11_m7	ring statistics, density of 11 membered rings containing 7 C atoms
C_n11_m8	ring statistics, density of 11 membered rings containing 8 C atoms
C_n11_m9	ring statistics, density of 11 membered rings containing 9 C atoms
C_n12_m1	ring statistics, density of 12 membered rings containing 1 C atoms
C_n12_m10	ring statistics, density of 12 membered rings containing 10 C atoms
C_n12_m11	ring statistics, density of 12 membered rings containing 11 C atoms
C_n12_m12	ring statistics, density of 12 membered rings containing 12 C atoms
C_n12_m2	ring statistics, density of 12 membered rings containing 2 C atoms
C_n12_m3	ring statistics, density of 12 membered rings containing 3 C atoms
C_n12_m4	ring statistics, density of 12 membered rings containing 4 C atoms
C_n12_m5	ring statistics, density of 12 membered rings containing 5 C atoms
C_n12_m6	ring statistics, density of 12 membered rings containing 6 C atoms
C_n12_m7	ring statistics, density of 12 membered rings containing 7 C atoms
C_n12_m8	ring statistics, density of 12 membered rings containing 8 C atoms
C_n12_m9	ring statistics, density of 12 membered rings containing 9 C atoms
C_n3_m1	ring statistics, density of 3 membered rings containing 1 C atoms
C_n3_m2	ring statistics, density of 3 membered rings containing 2 C atoms
C_n3_m3	ring statistics, density of 3 membered rings containing 3 C atoms
C_n4_m1	ring statistics, density of 4 membered rings containing 1 C atoms
C_n4_m2	ring statistics, density of 4 membered rings containing 2 C atoms
C_n4_m3	ring statistics, density of 4 membered rings containing 3 C atoms
C_n4_m4	ring statistics, density of 4 membered rings containing 4 C atoms
C_n5_m1	ring statistics, density of 5 membered rings containing 1 C atoms
C_n5_m2	ring statistics, density of 5 membered rings containing 2 C atoms
C_n5_m3	ring statistics, density of 5 membered rings containing 3 C atoms
C_n5_m4	ring statistics, density of 5 membered rings containing 4 C atoms

Continued on next page

Column	Description
C_n5_m5	ring statistics, density of 5 membered rings containing 5 C atoms
C_n6_m1	ring statistics, density of 6 membered rings containing 1 C atoms
C_n6_m2	ring statistics, density of 6 membered rings containing 2 C atoms
C_n6_m3	ring statistics, density of 6 membered rings containing 3 C atoms
C_n6_m4	ring statistics, density of 6 membered rings containing 4 C atoms
C_n6_m5	ring statistics, density of 6 membered rings containing 5 C atoms
C_n6_m6	ring statistics, density of 6 membered rings containing 6 C atoms
C_n7_m1	ring statistics, density of 7 membered rings containing 1 C atoms
C_n7_m2	ring statistics, density of 7 membered rings containing 2 C atoms
C_n7_m3	ring statistics, density of 7 membered rings containing 3 C atoms
C_n7_m4	ring statistics, density of 7 membered rings containing 4 C atoms
C_n7_m5	ring statistics, density of 7 membered rings containing 5 C atoms
C_n7_m6	ring statistics, density of 7 membered rings containing 6 C atoms
C_n7_m7	ring statistics, density of 7 membered rings containing 7 C atoms
C_n8_m1	ring statistics, density of 8 membered rings containing 1 C atoms
C_n8_m2	ring statistics, density of 8 membered rings containing 2 C atoms
C_n8_m3	ring statistics, density of 8 membered rings containing 3 C atoms
C_n8_m4	ring statistics, density of 8 membered rings containing 4 C atoms
C_n8_m5	ring statistics, density of 8 membered rings containing 5 C atoms
C_n8_m6	ring statistics, density of 8 membered rings containing 6 C atoms
C_n8_m7	ring statistics, density of 8 membered rings containing 7 C atoms
C_n8_m8	ring statistics, density of 8 membered rings containing 8 C atoms
C_n9_m1	ring statistics, density of 9 membered rings containing 1 C atoms
C_n9_m2	ring statistics, density of 9 membered rings containing 2 C atoms
C_n9_m3	ring statistics, density of 9 membered rings containing 3 C atoms
C_n9_m4	ring statistics, density of 9 membered rings containing 4 C atoms
C_n9_m5	ring statistics, density of 9 membered rings containing 5 C atoms
C_n9_m6	ring statistics, density of 9 membered rings containing 6 C atoms
C_n9_m7	ring statistics, density of 9 membered rings containing 7 C atoms
C_n9_m8	ring statistics, density of 9 membered rings containing 8 C atoms
C_n9_m9	ring statistics, density of 9 membered rings containing 9 C atoms
H-C_coordination_number	H-C average coordination numbers of first neighbours
H-O_coordination_number	H-O average coordination numbers of first neighbours
O-C_coordination_number	O-C average coordination numbers of first neighbours
O-H_coordination_number	O-H average coordination numbers of first neighbours
O-O_-coordination_number	O-O average coordination numbers of first neighbours
O_atoms_only_1_neighbourtotal	total number of O atoms with only 1 neighbour
O_atoms_with_bond_angles_-<_90_deg._total	total number of O atoms with bond angles deg <90 deg.
O_n10_m1	ring statistics, density of 10 membered rings containing 1 O atoms
O_n10_m10	ring statistics, density of 10 membered rings containing 10 O atoms
O_n10_m2	ring statistics, density of 10 membered rings containing 2 O atoms
O_n10_m3	ring statistics, density of 10 membered rings containing 3 O atoms
O_n10_m4	ring statistics, density of 10 membered rings containing 4 O atoms
O_n10_m5	ring statistics, density of 10 membered rings containing 5 O atoms
O_n10_m6	ring statistics, density of 10 membered rings containing 6 O atoms
O_n10_m7	ring statistics, density of 10 membered rings containing 7 O atoms
O_n10_m8	ring statistics, density of 10 membered rings containing 8 O atoms

Continued on next page

Column	Description
O_n10_m9	ring statistics, density of 10 membered rings containing 9 O atoms
O_n11_m1	ring statistics, density of 11 membered rings containing 1 O atoms
O_n11_m10	ring statistics, density of 11 membered rings containing 10 O atoms
O_n11_m11	ring statistics, density of 11 membered rings containing 11 O atoms
O_n11_m2	ring statistics, density of 11 membered rings containing 2 O atoms
O_n11_m3	ring statistics, density of 11 membered rings containing 3 O atoms
O_n11_m4	ring statistics, density of 11 membered rings containing 4 O atoms
O_n11_m5	ring statistics, density of 11 membered rings containing 5 O atoms
O_n11_m6	ring statistics, density of 11 membered rings containing 6 O atoms
O_n11_m7	ring statistics, density of 11 membered rings containing 7 O atoms
O_n11_m8	ring statistics, density of 11 membered rings containing 8 O atoms
O_n11_m9	ring statistics, density of 11 membered rings containing 9 O atoms
O_n12_m1	ring statistics, density of 12 membered rings containing 1 O atoms
O_n12_m10	ring statistics, density of 12 membered rings containing 10 O atoms
O_n12_m11	ring statistics, density of 12 membered rings containing 11 O atoms
O_n12_m12	ring statistics, density of 12 membered rings containing 12 O atoms
O_n12_m2	ring statistics, density of 12 membered rings containing 2 O atoms
O_n12_m3	ring statistics, density of 12 membered rings containing 3 O atoms
O_n12_m4	ring statistics, density of 12 membered rings containing 4 O atoms
O_n12_m5	ring statistics, density of 12 membered rings containing 5 O atoms
O_n12_m6	ring statistics, density of 12 membered rings containing 6 O atoms
O_n12_m7	ring statistics, density of 12 membered rings containing 7 O atoms
O_n12_m8	ring statistics, density of 12 membered rings containing 8 O atoms
O_n12_m9	ring statistics, density of 12 membered rings containing 9 O atoms
O_n3_m1	ring statistics, density of 3 membered rings containing 1 O atoms
O_n3_m2	ring statistics, density of 3 membered rings containing 2 O atoms
O_n3_m3	ring statistics, density of 3 membered rings containing 3 O atoms
O_n4_m1	ring statistics, density of 4 membered rings containing 1 O atoms
O_n4_m2	ring statistics, density of 4 membered rings containing 2 O atoms
O_n4_m3	ring statistics, density of 4 membered rings containing 3 O atoms
O_n4_m4	ring statistics, density of 4 membered rings containing 4 O atoms
O_n5_m1	ring statistics, density of 5 membered rings containing 1 O atoms
O_n5_m2	ring statistics, density of 5 membered rings containing 2 O atoms
O_n5_m3	ring statistics, density of 5 membered rings containing 3 O atoms
O_n5_m4	ring statistics, density of 5 membered rings containing 4 O atoms
O_n5_m5	ring statistics, density of 5 membered rings containing 5 O atoms
O_n6_m1	ring statistics, density of 6 membered rings containing 1 O atoms
O_n6_m2	ring statistics, density of 6 membered rings containing 2 O atoms
O_n6_m3	ring statistics, density of 6 membered rings containing 3 O atoms
O_n6_m4	ring statistics, density of 6 membered rings containing 4 O atoms
O_n6_m5	ring statistics, density of 6 membered rings containing 5 O atoms
O_n6_m6	ring statistics, density of 6 membered rings containing 6 O atoms
O_n7_m1	ring statistics, density of 7 membered rings containing 1 O atoms
O_n7_m2	ring statistics, density of 7 membered rings containing 2 O atoms
O_n7_m3	ring statistics, density of 7 membered rings containing 3 O atoms
O_n7_m4	ring statistics, density of 7 membered rings containing 4 O atoms
O_n7_m5	ring statistics, density of 7 membered rings containing 5 O atoms
O_n7_m6	ring statistics, density of 7 membered rings containing 6 O atoms

Continued on next page

Column	Description
O_n7_m7	ring statistics, density of 7 membered rings containing 7 O atoms
O_n8_m1	ring statistics, density of 8 membered rings containing 1 O atoms
O_n8_m2	ring statistics, density of 8 membered rings containing 2 O atoms
O_n8_m3	ring statistics, density of 8 membered rings containing 3 O atoms
O_n8_m4	ring statistics, density of 8 membered rings containing 4 O atoms
O_n8_m5	ring statistics, density of 8 membered rings containing 5 O atoms
O_n8_m6	ring statistics, density of 8 membered rings containing 6 O atoms
O_n8_m7	ring statistics, density of 8 membered rings containing 7 O atoms
O_n8_m8	ring statistics, density of 8 membered rings containing 8 O atoms
O_n9_m1	ring statistics, density of 9 membered rings containing 1 O atoms
O_n9_m2	ring statistics, density of 9 membered rings containing 2 O atoms
O_n9_m3	ring statistics, density of 9 membered rings containing 3 O atoms
O_n9_m4	ring statistics, density of 9 membered rings containing 4 O atoms
O_n9_m5	ring statistics, density of 9 membered rings containing 5 O atoms
O_n9_m6	ring statistics, density of 9 membered rings containing 6 O atoms
O_n9_m7	ring statistics, density of 9 membered rings containing 7 O atoms
O_n9_m8	ring statistics, density of 9 membered rings containing 8 O atoms
O_n9_m9	ring statistics, density of 9 membered rings containing 9 O atoms
ring_density_10_irreducible_sp	density of irreducible (sp) 10 membered rings
ring_density_10_reducible_all	density of reducible (all) 10 membered rings
ring_density_11_irreducible_sp	density of irreducible (sp) 11 membered rings
ring_density_11_reducible_all	density of reducible (all) 11 membered rings
ring_density_12_irreducible_sp	density of irreducible (sp) 12 membered rings
ring_density_12_reducible_all	density of reducible (all) 12 membered rings
ring_density_3_irreducible_sp	density of irreducible (sp) 3 membered rings
ring_density_3_reducible_all	density of reducible (all) 3 membered rings
ring_density_4_irreducible_sp	density of irreducible (sp) 4 membered rings
ring_density_4_reducible_all	density of reducible (all) 4 membered rings
ring_density_5_irreducible_sp	density of irreducible (sp) 5 membered rings
ring_density_5_reducible_all	density of reducible (all) 5 membered rings
ring_density_6_irreducible_sp	density of irreducible (sp) 6 membered rings
ring_density_6_reducible_all	density of reducible (all) 6 membered rings
ring_density_7_irreducible_sp	density of irreducible (sp) 7 membered rings
ring_density_7_reducible_all	density of reducible (all) 7 membered rings
ring_density_8_irreducible_sp	density of irreducible (sp) 8 membered rings
ring_density_8_reducible_all	density of reducible (all) 8 membered rings
ring_density_9_irreducible_sp	density of irreducible (sp) 9 membered rings
ring_density_9_reducible_all	density of reducible (all) 9 membered rings
rings_total_number_10_all	the total number of reducible (all) 10 membered rings
rings_total_number_10_sp	the total number of irreducible (sp) 10 membered rings
rings_total_number_11_all	the total number of reducible (all) 11 membered rings
rings_total_number_11_sp	the total number of irreducible (sp) 11 membered rings
rings_total_number_12_all	the total number of reducible (all) 12 membered rings
rings_total_number_12_sp	the total number of irreducible (sp) 12 membered rings
rings_total_number_3_all	the total number of reducible (all) 3 membered rings
rings_total_number_3_sp	the total number of irreducible (sp) 3 membered rings
rings_total_number_4_all	the total number of reducible (all) 4 membered rings
rings_total_number_4_sp	the total number of irreducible (sp) 4 membered rings

Continued on next page

Column	Description
rings_total_number_5_all	the total number of reducible (all) 5 membered rings
rings_total_number_5_sp	the total number of irreducible (sp) 5 membered rings
rings_total_number_6_all	the total number of reducible (all) 6 membered rings
rings_total_number_6_sp	the total number of irreducible (sp) 6 membered rings
rings_total_number_7_all	the total number of reducible (all) 7 membered rings
rings_total_number_7_sp	the total number of irreducible (sp) 7 membered rings
rings_total_number_8_all	the total number of reducible (all) 8 membered rings
rings_total_number_8_sp	the total number of irreducible (sp) 8 membered rings
rings_total_number_9_all	the total number of reducible (all) 9 membered rings
rings_total_number_9_sp	the total number of irreducible (sp) 9 membered rings
sp2-like_n10_m1	ring statistics, density of 10 membered rings containing 1 sp2-like atoms
sp2-like_n10_m10	ring statistics, density of 10 membered rings containing 10 sp2-like atoms
sp2-like_n10_m2	ring statistics, density of 10 membered rings containing 2 sp2-like atoms
sp2-like_n10_m3	ring statistics, density of 10 membered rings containing 3 sp2-like atoms
sp2-like_n10_m4	ring statistics, density of 10 membered rings containing 4 sp2-like atoms
sp2-like_n10_m5	ring statistics, density of 10 membered rings containing 5 sp2-like atoms
sp2-like_n10_m6	ring statistics, density of 10 membered rings containing 6 sp2-like atoms
sp2-like_n10_m7	ring statistics, density of 10 membered rings containing 7 sp2-like atoms
sp2-like_n10_m8	ring statistics, density of 10 membered rings containing 8 sp2-like atoms
sp2-like_n10_m9	ring statistics, density of 10 membered rings containing 9 sp2-like atoms
sp2-like_n11_m1	ring statistics, density of 11 membered rings containing 1 sp2-like atoms
sp2-like_n11_m10	ring statistics, density of 11 membered rings containing 10 sp2-like atoms
sp2-like_n11_m11	ring statistics, density of 11 membered rings containing 11 sp2-like atoms
sp2-like_n11_m2	ring statistics, density of 11 membered rings containing 2 sp2-like atoms
sp2-like_n11_m3	ring statistics, density of 11 membered rings containing 3 sp2-like atoms
sp2-like_n11_m4	ring statistics, density of 11 membered rings containing 4 sp2-like atoms
sp2-like_n11_m5	ring statistics, density of 11 membered rings containing 5 sp2-like atoms
sp2-like_n11_m6	ring statistics, density of 11 membered rings containing 6 sp2-like atoms
sp2-like_n11_m7	ring statistics, density of 11 membered rings containing 7 sp2-like atoms
sp2-like_n11_m8	ring statistics, density of 11 membered rings containing 8 sp2-like atoms
sp2-like_n11_m9	ring statistics, density of 11 membered rings containing 9 sp2-like atoms
sp2-like_n12_m1	ring statistics, density of 12 membered rings containing 1 sp2-like atoms
sp2-like_n12_m10	ring statistics, density of 12 membered rings containing 10 sp2-like atoms
sp2-like_n12_m11	ring statistics, density of 12 membered rings containing 11 sp2-like atoms
sp2-like_n12_m12	ring statistics, density of 12 membered rings containing 12 sp2-like atoms
sp2-like_n12_m2	ring statistics, density of 12 membered rings containing 2 sp2-like atoms
sp2-like_n12_m3	ring statistics, density of 12 membered rings containing 3 sp2-like atoms
sp2-like_n12_m4	ring statistics, density of 12 membered rings containing 4 sp2-like atoms
sp2-like_n12_m5	ring statistics, density of 12 membered rings containing 5 sp2-like atoms
sp2-like_n12_m6	ring statistics, density of 12 membered rings containing 6 sp2-like atoms
sp2-like_n12_m7	ring statistics, density of 12 membered rings containing 7 sp2-like atoms
sp2-like_n12_m8	ring statistics, density of 12 membered rings containing 8 sp2-like atoms
sp2-like_n12_m9	ring statistics, density of 12 membered rings containing 9 sp2-like atoms
sp2-like_n3_m1	ring statistics, density of 3 membered rings containing 1 sp2-like atoms
sp2-like_n3_m2	ring statistics, density of 3 membered rings containing 2 sp2-like atoms
sp2-like_n3_m3	ring statistics, density of 3 membered rings containing 3 sp2-like atoms
sp2-like_n4_m1	ring statistics, density of 4 membered rings containing 1 sp2-like atoms
sp2-like_n4_m2	ring statistics, density of 4 membered rings containing 2 sp2-like atoms

Continued on next page

Column	Description
sp2-like_n4_m3	ring statistics, density of 4 membered rings containing 3 sp2-like atoms
sp2-like_n4_m4	ring statistics, density of 4 membered rings containing 4 sp2-like atoms
sp2-like_n5_m1	ring statistics, density of 5 membered rings containing 1 sp2-like atoms
sp2-like_n5_m2	ring statistics, density of 5 membered rings containing 2 sp2-like atoms
sp2-like_n5_m3	ring statistics, density of 5 membered rings containing 3 sp2-like atoms
sp2-like_n5_m4	ring statistics, density of 5 membered rings containing 4 sp2-like atoms
sp2-like_n5_m5	ring statistics, density of 5 membered rings containing 5 sp2-like atoms
sp2-like_n6_m1	ring statistics, density of 6 membered rings containing 1 sp2-like atoms
sp2-like_n6_m2	ring statistics, density of 6 membered rings containing 2 sp2-like atoms
sp2-like_n6_m3	ring statistics, density of 6 membered rings containing 3 sp2-like atoms
sp2-like_n6_m4	ring statistics, density of 6 membered rings containing 4 sp2-like atoms
sp2-like_n6_m5	ring statistics, density of 6 membered rings containing 5 sp2-like atoms
sp2-like_n6_m6	ring statistics, density of 6 membered rings containing 6 sp2-like atoms
sp2-like_n7_m1	ring statistics, density of 7 membered rings containing 1 sp2-like atoms
sp2-like_n7_m2	ring statistics, density of 7 membered rings containing 2 sp2-like atoms
sp2-like_n7_m3	ring statistics, density of 7 membered rings containing 3 sp2-like atoms
sp2-like_n7_m4	ring statistics, density of 7 membered rings containing 4 sp2-like atoms
sp2-like_n7_m5	ring statistics, density of 7 membered rings containing 5 sp2-like atoms
sp2-like_n7_m6	ring statistics, density of 7 membered rings containing 6 sp2-like atoms
sp2-like_n7_m7	ring statistics, density of 7 membered rings containing 7 sp2-like atoms
sp2-like_n8_m1	ring statistics, density of 8 membered rings containing 1 sp2-like atoms
sp2-like_n8_m2	ring statistics, density of 8 membered rings containing 2 sp2-like atoms
sp2-like_n8_m3	ring statistics, density of 8 membered rings containing 3 sp2-like atoms
sp2-like_n8_m4	ring statistics, density of 8 membered rings containing 4 sp2-like atoms
sp2-like_n8_m5	ring statistics, density of 8 membered rings containing 5 sp2-like atoms
sp2-like_n8_m6	ring statistics, density of 8 membered rings containing 6 sp2-like atoms
sp2-like_n8_m7	ring statistics, density of 8 membered rings containing 7 sp2-like atoms
sp2-like_n8_m8	ring statistics, density of 8 membered rings containing 8 sp2-like atoms
sp2-like_n9_m1	ring statistics, density of 9 membered rings containing 1 sp2-like atoms
sp2-like_n9_m2	ring statistics, density of 9 membered rings containing 2 sp2-like atoms
sp2-like_n9_m3	ring statistics, density of 9 membered rings containing 3 sp2-like atoms
sp2-like_n9_m4	ring statistics, density of 9 membered rings containing 4 sp2-like atoms
sp2-like_n9_m5	ring statistics, density of 9 membered rings containing 5 sp2-like atoms
sp2-like_n9_m6	ring statistics, density of 9 membered rings containing 6 sp2-like atoms
sp2-like_n9_m7	ring statistics, density of 9 membered rings containing 7 sp2-like atoms
sp2-like_n9_m8	ring statistics, density of 9 membered rings containing 8 sp2-like atoms
sp2-like_n9_m9	ring statistics, density of 9 membered rings containing 9 sp2-like atoms
r_OO_mean	average distance between oxygen atoms
r_ether_ether_mean	average distance between ether groups
r_hydro_hydro_mean	average distance between hydroxyl groups
r_ether_hydro_mean	average inter-distance between ether and hydroxyl groups
r_OO_std	standard deviation in distance between oxygen atoms
r_ether_ether_std	standard deviation in distance between ether groups
r_hydro_hydro_std	standard deviation in distance between hydroxyl groups
r_ether_hydro_std	standard deviation in inter-distance between ether and hydroxyl groups
density_loc_C_mean	average of local densities of carbon atoms
density_loc_O_mean	average of local densities of oxygen atoms
density_loc_ether_mean	average of local densities of ether groups
density_loc_hydro_mean	average of local densities of hydroxyl groups

Continued on next page

Column	Description
hline density_loc_C_min	minimum local densities of carbon atoms
density_loc_O_min	minimum local densities of oxygen atoms
density_loc_ether_min	minimum local densities of ether groups
density_loc_hydro_min	minimum local densities of hydroxyl groups
hline density_loc_C_max	maximum local densities of carbon atoms
density_loc_O_max	maximum local densities of oxygen atoms
density_loc_ether_max	maximum local densities of ether groups
density_loc_hydro_max	maximum local densities of hydroxyl groups
density_loc_C_std	standard deviation in local density distribution of carbon atoms
density_loc_O_std	standard deviation in local density distribution of oxygen atoms
density_loc_ether_std	standard deviation in local density distribution of ether groups
density_loc_hydro_std	standard deviation in local density distribution of hydroxyl groups
density_loc_C_skew	skewness in local density distribution of carbon atoms
density_loc_O_skew	skewness in local density distribution of oxygen atoms
density_loc_ether_skew	skewness in local density distribution of ether groups
density_loc_hydro_skew	skewness in local density distribution of hydroxyl groups
density_loc_C_kurt	kurtosis in local density distribution of carbon atoms
density_loc_O_kurt	kurtosis in local density distribution of oxygen atoms
density_loc_ether_kurt	kurtosis in local density distribution of ether groups
density_loc_hydro_kurt	kurtosis in local density distribution of hydroxyl groups
norm_density_O_mean	average of normalised local densities of oxygen atoms
norm_density_ether_mean	average of normalised local densities of ether groups
norm_density_hydro_mean	average of normalised local densities of hydroxyl groups
norm_density_O_min	minimum normalised local densities of oxygen atoms
norm_density_ether_min	minimum normalised local densities of ether groups
norm_density_hydro_min	minimum normalised local densities of hydroxyl groups
norm_density_O_max	maximum normalised local densities of oxygen atoms
norm_density_ether_max	maximum normalised local densities of ether groups
norm_density_hydro_max	maximum normalised local densities of hydroxyl groups
norm_density_O_std	standard deviation in normalised local densities of oxygen atoms
norm_density_ether_std	standard deviation in of normalised local densities of ether groups
norm_density_hydro_std	standard deviation in of normalised local densities of hydroxyl groups
norm_density_O_skew	skewness in normalised local densities of oxygen atoms
norm_density_ether_skew	skewness in of normalised local densities of ether groups
norm_density_hydro_skew	skewness in of normalised local densities of hydroxyl groups
norm_density_O_kurt	kurtosis in normalised local densities of oxygen atoms
norm_density_ether_kurt	kurtosis in of normalised local densities of ether groups
norm_density_hydro_kurt	kurtosis in of normalised local densities of hydroxyl groups
PROPERTY LABELS	
total_energy	total energy of the entire nanoflake, in eV
Fermi_energy	the energy of the Fermi level of the nanoflake, in eV

References

(1) B. Aradi, B. Hourahine, Th. Frauenheim, *J. Phys. Chem. A*, **111**, (2007) 5678

(2) Th. Frauenheim, G. Seifert, M. Elstner, Th. Niehaus, C. Köhler, M. Amkreutz, M. Sternberg, Z. Hajnal, A. Di Carlo, S. Suhai, *J. Phys.: Condens. Matter* **14** (2002) 3015

(3) D. Porezag, Th. Frauenheim, Th. Köhler, G. Seifert, R. Kaschner, *Phys. Rev. B* **51** (1995) 12947

(4) A. Castro Neto, F. Guinea, N. M. R. Peres, K. Novoselov, A. Geim, *Rev. Mod. Phys.* **81** (2009) 109

(5) P. Phillips, *Ann. Phys.* **321** (2006) 1634.

(6) S. Reich, J. Maultzsch, C. Thomsen, P. Ordejón, *Phys. Rev. B* **66** (2002) 035412

(7) A. Zobelli, V. Ivanovskaya, P. Wagner, I. Suarez-Martinez, A. Yaya, C. P. Ewels, *Physica Status Solidi (b)* **249** (2012) 276.

(8) M. Fernandez, A. Bilić, A. S. Barnard, *Nanotech.* **28** (2017) 38LT03

(9) C. Köhler, T. Frauenheim, *Surf. Sci.* **600** (2006) 453.

(10) A. S. Barnard, M. Sternberg, *J. Mater. Chem.* **17** (2007) 4811

(11) L. Y. Chang, E. Ōsawa, A. S. Barnard, *Nanoscale*, **3** (2011) 958

(12) A. S. Barnard, I. K. Snook, *Model. Simul. Mater. Sci. Eng.* **19** (2011) 054001

(13) L. Lai, A. S. Barnard, *Nanoscale*, **3** (2011) 2566

(14) H. Shi, A. S. Barnard, I. K. Snook, *Nanotech.* **23** (2012) 065707

(15) H. Shi, A. S. Barnard, I. K. Snook, *J. Mater. Chem.* **22** (2012) 18119

(16) H. Q. Shi, A. S. Barnard, I.K. Snook, *Nanoscale* **4**, (2012) 6761

(17) L. Lai, A. S. Barnard, *J. Phys. Chem. C*, **115** (2011) 6218

(18) H. Q. Shi, I. K. Snook, A. S. Barnard, *Phys. Chem. Chem. Phys.* **15** (2013) 4897

(19) H. Q. Shi, L. Lai, I. K. Snook, A. S. Barnard, *J. Phys. Chem. C* **117** (2013) 15375

(20) A. S. Barnard, *Nanotech.* **24** (2013) 085703

(21) L. Lai, A. S. Barnard, *Phys. Chem. Chem. Phys.* **15** (2013) 9156

(22) L. K. Randeniya, H. Q. Shi, A. S. Barnard, J. Fang, P. J. Martin, K. Ostrikov, *Small* **9**, (2013) 3993

(23) A. S. Barnard, *Mater. Horizons* **1** (2014) 289

(24) A. S. Barnard, M. C. Per, *Nanotech.* **25** (2014) 445702

(25) L. Lai, A. S. Barnard, *Nanoscale*, **6** (2014) 14185

(26) L. Lai, A. S. Barnard, *J. Phys. Chem. C*, **118** (2014) 30209

(27) L. Lai, A. S. Barnard, *J. Nanosci. Nanotech.* **15** (2015) 989

(28) H. Q. Shi, R. J. Rees, M. C. Per, A. S. Barnard, *Nanoscale*, **7** (2015) 1864

(29) M. C. Per, A. S. Barnard, I. K. Snook, *Molec. Simulat.* **42** (2016) 458

(30) L. Lai, A. S. Barnard, *Nanoscale* **8** (2016) 7899

(31) S. L. Y. Chang, A. S. Barnard, C. Dwyer, C. B. Boothroyd, R. Hocking, E. Ōsawa, R. J. Nicholls, *Nanoscale* **19** (2016) 10548

(32) A. S. Barnard, *Nanoscale* **9** (2017) 70

(33) S. L. Y. Chang, C. Dwyer, K. March, M. Mermoux, N. Nunn, O. Shenderova, E. Osawa, A. S. Barnard, *Micros. Microanal.* **23** (2017) 2270

(34) S. L. Y. Chang, C. Dwyer, E. Ōsawa, A. S. Barnard, *Nanoscale Horiz.* **3** (2018) 213

(35) A. S. Barnard, *Nanoscale* **10** (2018) 8893

(36) D. Abergel, V. Apalkov, J. Berashevich, K. Zieler, T. Chakraborty, *Adv. Phys.* **59** (2010) 261

(37) V. Barone, O. Hod, E. Scuseria, *Nano Lett.* **6** (2006) 2748

(38) Y. Son, M. Cohen, S. Louie, *Nature*, **444** (2006) 347

(39) Y. Son, M. Cohen and S. Louie, *Phys. Rev. Lett.* **97** (2006) 216803

(40) A. S. Barnard, I. K. Snook, *Carbon*, **48** (2010) 98.

(41) A. S. Barnard, I. K. Snook, *J. Mater. Chem.* **20** (2010) 10459

(42) L. Lai, A. S. Barnard, *Nanoscale*, **3** (2011) 2566

(43) L. Lai, A. S. Barnard, *J. Mater. Chem.* **22** (2012) 13141

(44) M. Fernandez, H. Q. Shi, A. S. Barnard, *J. Chem. Info. Mod.* **55**, (2015) 2500

(45) M. Fernandez, A. S. Barnard, *ACS Nano* **9** (2015) 11980

(46) M. Fernandez, J. I. Abreu, H. Q. Shi, A. S. Barnard, *ACS Combi. Sci.* **18** (2016) 661

(47) M. Fernandez, H. Q. Shi, A. S. Barnard, *Carbon* **103** (2016) 142