Corrigendum

Corrigendum to "Study of the cap structure of (3,3), (4,4) and (5,5)-SWCNTs: Application of the sphere-in-contact model" [Carbon 115 (2017) 819–827]

Constantinos D. Zeinalipour-Yazdi [a, *], Eriketi Z. Loizidou [b]

[a] Kathleen Lonsdale Materials Chemistry, Department of Chemistry, University College London, London, WC1H 0AJ, UK
[b] Department of Natural Sciences, Middlesex University, Hendon Campus, The Burroughs, London, NW4 4BT, UK

The authors regret that the printed version of the above article contained four incorrect signs in Eqn. (5) which caused the BDE to become negative. The correct and final version follows. The authors would like to apologise for any inconvenience caused.

The change in enthalpy for the bond formation of a PAH from its atoms was calculated based on the following equation

$$\Delta H \cong E_{PAH} - n_C E_C - n_H E_H + ZPV_{PAH} \tag{1}$$

where n_C and n_H is the number of C and H atoms, respectively. E_{PAH}, E_C and E_H are the total energies of the PAH, of an isolated carbon atom in its triplet state and a hydrogen atom in its doublet state and the zero-point vibrational energy (ZPV_{PAH}) was calculated based on,

$$ZPV_{PAH} \cong \frac{hc}{2} \left(\sum_{i=1}^{n_{CC}} \nu_{CC,i} + \sum_{j=1}^{n_{CH}} \nu_{CH,j} \right), \tag{2}$$

where n_{CC} and n_{CH} are the number of C–C and C–H bonds, respectively. Furthermore $\nu_{CC,i}$ and $\nu_{CH,j}$ are the vibrational frequencies of the bonds i and j, respectively, which were calculated via the harmonic oscillator approximation and the finite-difference method. The enthalpy of atomization of the PAH was calculated based on the following relationship,

$$\Delta H_{atom} = n_{CC} BDE_{CC} + n_{CH} BDE_{CH}, \tag{3}$$

where BDE_{CH} and BDE_{CC} are the average bond-dissociation energies of the C–H bond and C–C bond, respectively. The change in enthalpy for the bond formation of the PAH is equal to the negative atomization enthalpy,

$$\Delta H = -\Delta H_{atom}. \tag{4}$$

Therefore after combination of equations (1)–(4), the average BDE per C–C bond in an arbitrary PAH becomes,

$$BDE_{CC} \cong \frac{1}{n_{CC}} \left[-E_{PAH} + n_C E_C + n_H E_H - \frac{hc}{2} \left(\sum_{i=1}^{n_{CC}} \nu_{CC,i} + \sum_{j=1}^{n_{CH}} \nu_{CH,j} \right) - n_{CH} BDE_{CH} \right]. \tag{5}$$

The BDE_{CH} was estimated based on the energy required to dissociate a hydrogen atom from coronene ($R = C_{24}H_{12}$) forming the corresponding radical ($R^\bullet = C_{24}H_{11}{}^\bullet$) given by,

$$BDE_{CH} = E_{RH} - E_{R^\bullet} - E_{H^+} + ZPV_{CH}. \tag{6}$$

The average BDE_{CH} for coronene at B3YP/cc-pVDZ(5d,7f) level of theory was found to be 454 kJ mol^{-1} comparable to value reported for the BDE_{CH} in benzene 473 kJ mol^{-1} and methane 439 kJ mol^{-1}. [28] The zero-point vibrational energy (ZPV) of C–H at the same level of theory was found to be 34 kJ mol^{-1} in excellent agreement with the zero-point energy (ZPE) 36 kJ mol^{-1}, calculated from the IR band of the C–H stretching in PAHs located between 3000 and 3100cm^{-1} [29], with the formula given by,

$$ZPE = \hbar \frac{\omega}{2}.$$ (7)

The ZPV of C–H was calculated with the following equation,

$$ZPV_{CH} = ZPV_{RH} - ZPV_{R\bullet},$$

where ZPV_{RH} and $ZPV_{R\bullet}$. are the zero-point vibrational energies of coronene and coronene radical in its triplet state calculated at B3YP/cc-pVDZ(5d,7f), respectively.

The average BDE_{CH} of various stable carbon structures and the capped-SWCNT are shown Fig. 6. These calculations show that the stability of planar carbon materials is higher than carbon materials with curved surfaces (e.g. Fullerenes, NC and CNTs). This is associated to the existence of the energy requirements to bend GNR.[30] The bending energy is considerable smaller that the shearing and compression energy as we have previously shown for GNR of varying size. [30] Noteworthy, is that the average BDE_{CC} is correlated to the degree of curvature of the materials shown in Fig. 6. GNR has the highest BDE_{CC} due to its planar structure. This is followed by nanocones (NC) whose energy increases inversely proportional to the tip angle, defined by one of the vertical mirror planes of the C_{5v} and C_{4v}, point group symmetries, respectively. The stability of the capped-SWCNT we have examined is intermediate between that of fullerene and the NCs. The most stable capped-SWCNT based on the calculated BDE was the capped (3,3)-SWCNT whereas the least stable was the capped (4,4)-SWCNT due to square geometry at the tip apex.
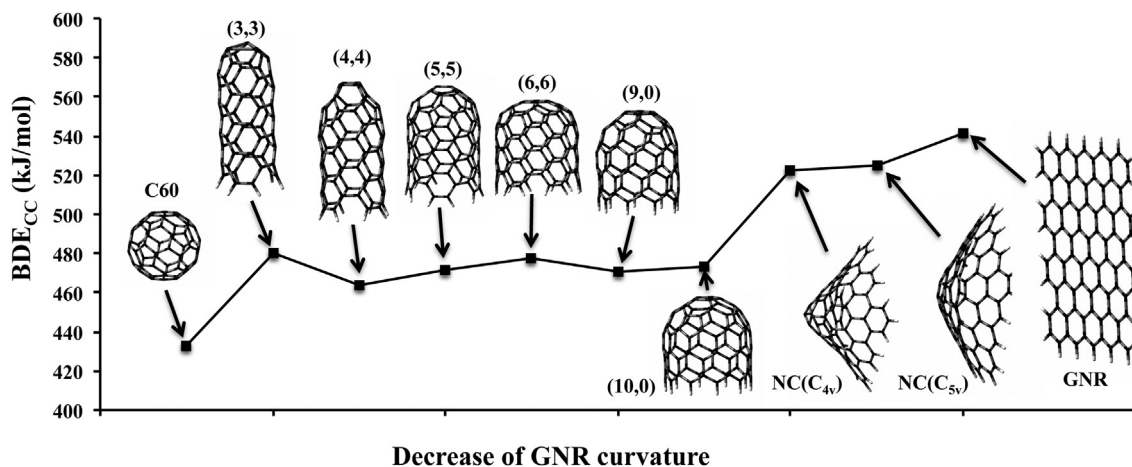

Decrease of GNR curvature

Fig. 6 Stability trends of various carbon materials based on the bond dissociation enthalpy of the C-C bond (BDE_{CC}) calculated by Eqn. (5) as a function of their curvature. Calculations made at B3LYP/cc-pVDZ level of theory.