Angewandte Chemie
Eine Zeitschrift der Gesellschaft Deutscher Chemiker

Supporting Information

Homo Citans and Carbon Allotropes: For an Ethics of Citation

Roald Hoffmann, Artyom A. Kabanov, Andrey A. Golov, and Davide M. Proserpio**

anie_201600655_sm_miscellaneous_information.pdf

SUPPORTING INFORMATION

1. SACADA: What the website presents.

All the parameters reported in the database are collected in 17 columns:

1. ***N.*** Serial number of the structure assigned to all chemically distinct allotropes: for example we have 4 entries for the underlying net of diamond **dia** that is associated also to the so called yne-diamond where for some or all bond there is a -C≡C- inserted, furthermore one of the latter (entry # 4, Y-II) is also 2-fold interpenetrated. The number is clickable if the net is included in the RCSR database, and will redirect to the appropriate RCSR page.

2. ***Topology.*** This column contains the name for the topology of the underlying net of each carbon allotrope. The abbreviations are clickable for downloading .tar.gz archives that contains two .cif files. One of them, with _IN suffix , corresponds to the net in maximal symmetry embedding (ideal nets with C-C bonds all equal to 1.00). The other, .cif, provides the DFT-optimized structure in maximal space group symmetry.

3. ***Space group.*** Space group of the ideal nets.

4. ***Number of Independent Nodes.*** Number of topological distinct nodes of the ideal nets.

5. ***CN (Ratio).*** The coordination number (CN) of nodes for ideal nets. The ratio between the numbers of nodes with different CN are shown in parentheses. The ratio is not shown if the numbers of nodes with different CN are equal. So e.g. for entry 2 the reported 2,4 means that there are 2-c and 4-connected nodes in equal ratio.

6. ***Pearson.*** The Pearson symbol of the ideal nets give information on the Bravais lattice and the total number of atoms in the unit cell. (see https://en.wikipedia.org/wiki/Pearson_symbol)

7. ***Transitivity.*** Transitivity of the tiling for the ideal net [pqrs], where p, q, r and s are numbers of inequivalent vertices, edges, faces and tiles in the tiling. This is a kind of measure of the complexity of the net.
See examples in "From zeolite nets to sp3 carbon allotropes: A topology-based multiscale theoretical study": I. A. Baburin, D. M. Proserpio, V. A. Saleev, A. V. Shipilova, *Phys. Chem. Chem. Phys.* **2015**, *17*, 1332 – 1338.

8. ***Names.*** All names of the carbon allotrope reported in the original literature for a given topology.

9. ***Pressure***. Pressure (GPa) at which the structure was computed.

10. ***Density*** . Density (g/cm³).

11. ***Gap***. Energy Band gap (eV).

12. ***Relative energy.*** Atomic energy relative to diamond (**eV/atom)**.

13. ***Bulk***. Bulk modulus (GPa).

14. ***Shear***. Shear modulus (GPa).

15. ***Vicker***. Vicker hardness (GPa).

16. ***Year.*** Year of the first report of the structure in the literature.

17. ***Refs.*** All references where each structure was reported. The references are arranged by years.

A searchable spread-sheet (.xls) file with all entries of the database (full references to 224 articles and all the reported values) is available at this link:

http://sacada.sctms.ru/files/SACADA_1march2016.xls

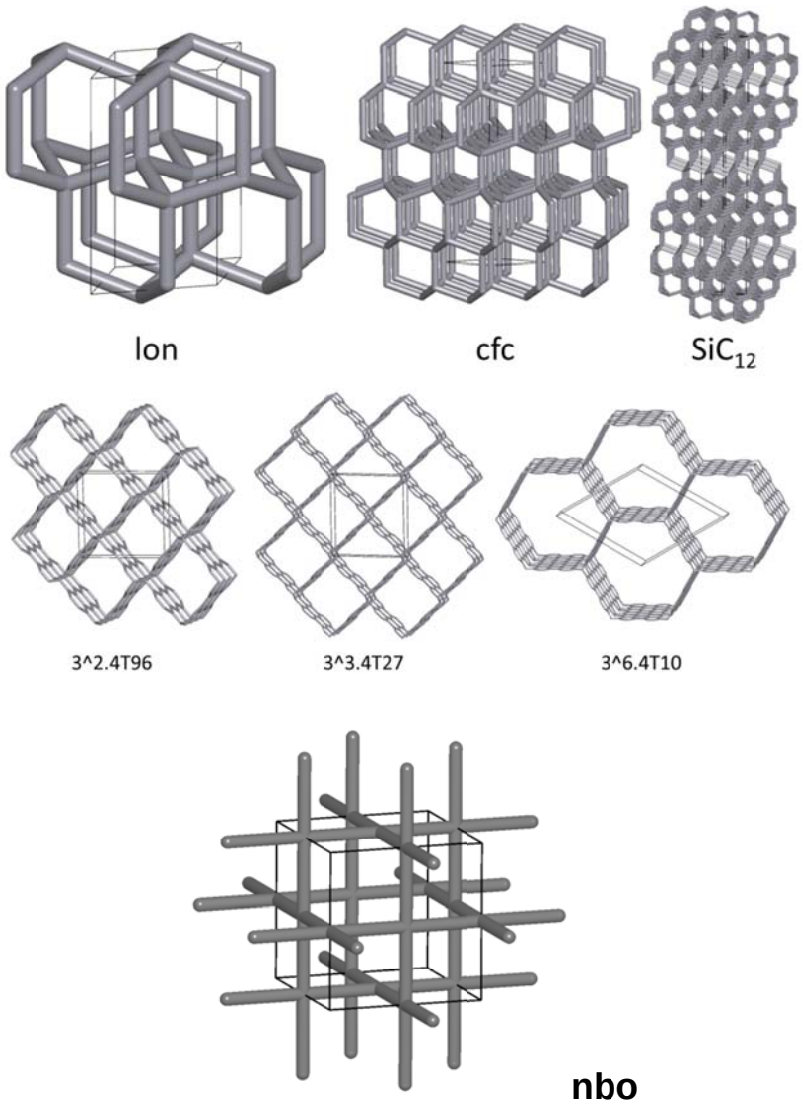

Figure S1. The six structures with the closest energy to diamond (less than 0.035 eV): three polytypes (top) and three "crossed graphene" sheets (middle), and **nbo**, the one with highest relative energy (bottom)