

## Corrigendum to "The simplest dense carbon allotrope: ultra-hard body-centered tetragonal C<sub>4</sub>"

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In our short communication [1] we reported the simplest dense carbon phase constructed from so called 'glitter' structure reproducing 1,4-cyclohexadiene molecule [2] using crystal chemistry rationale and geometry optimization onto ground state structures by DFT-based computations. The phase contains four carbon atoms in a body-centered tetragonal unit cell (space group  $I-4m2$ , No. 119) and is found to be as cohesive as diamond, and likewise built of corner sharing  $C4$  tetrahedra. Qualified as mechanically stable from the elastic constants combinations, the predicted phase has Vickers hardness identical to that of both cubic and hexagonal (lonsdaleite) diamond.

Further crystal symmetry analysis of the structure [3] revealed that the tetracarbon's announced space group  $I-4m2$  (No. 119) is inscribed in diamond's  $Fd-3m$  (No. 227) space group. Thus, we should admit that the body-centered tetragonal structure of the predicted carbon phase is another view of cubic diamond, described in a subgroup.

Looking back at our other recent work [4], we found that the predicted structure of rhombohedral ( $R-3m$ ) carbon is also another view of diamond. All this demonstrates the importance of thoroughly verifying theoretically predicted structures, which may be identical to the previously known ones [5] even when reported in different space groups.

It also shows that modeling a carbon structure that could compete with diamond (or its polytypes) in terms of mechanical properties is very difficult (or even impossible). Indeed, as it was previously stated, the hardness of diamond appears to be the theoretical limit for all possible materials [6-8].

The authors thank Prof. Davide M. Proserpio of Università degli Studi di Milano who pointed out the crystal symmetry problem and Prof. Artem R. Oganov of Skolkovo Institute of Science and Technology for valuable comments and suggestions.

## References

1. Matar SF, Solozhenko VL (2022) The simplest dense carbon allotrope: ultra-hard body centered tetragonal C<sub>4</sub>. *J. Solid State Chem.* **314**:123424.
2. Bucknum MJ, Hoffmann R (1994) A hypothetical dense 3,4-connected carbon net and related B<sub>2</sub>C and CN<sub>2</sub> nets built from 1,4-cyclohexadienoid units. *J. Am. Chem. Soc.* **116**:11456.
3. Müller U. Symmetry Relationships between Crystal Structures: Applications of Crystallographic Group Theory in Crystal Chemistry, Oxford: Oxford University Press; (2013).
4. Matar SF, Solozhenko VL (2021) Ultra-hard rhombohedral carbon by crystal chemistry and ab initio investigations. *J. Solid State Chem.* **302**:122354.
5. (a) Hoffmann R, Kabanov AA, Golov AA, Proserpio DM (2016) Homo Citans and carbon allotropes: For an ethics of citation. *Angew. Chem. Int. Ed.* **55**:10962-10976. (b) Samara Carbon Allotrope Database (<http://sacada.sctms.ru>)
6. Brazhkin VV, Solozhenko VL (2019) Myths about new ultrahard phases: Why materials that are significantly superior to diamond in elastic moduli and hardness are impossible. *J. Appl. Phys.* **125**:130901.
7. Avery P, Wang X, Oses C, Gossett E, Proserpio DM, Toher C, Curtarolo S, Zurek E (2019) Predicting superhard materials via a machine learning informed evolutionary structure search. *npj Comput. Mater.* **5**:89
8. Allahyari Z, Oganov AR (2020) Coevolutionary search for optimal materials in the space of all possible compounds. *npj Comput. Mater.* **6**:55