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Algorithmic Generation of Carbon Nanochimneys

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Abstract : Computational generation of carbon nanostructures is still a very demanding process. This work provides an alternative to manual molecular modeling through an algorithm meant to automate the design of such structures. Specifically, carbon nanochimneys are obtained through the bonding of a carbon nanotube with the smaller edge of an open carbon nanocone. The methods of connection rely on mathematical, geometrical and chemical properties. Non-hexagonal rings are used in order to perform the correct bonding of dangling bonds. Once obtained, they are useful for thermal transport, gas storage or other applications such as gas separation. The carbon nanochimneys are meant to produce a less steep connection between structures such as the carbon nanotube and graphene sheet, as in the pillared graphene, but can also provide functionality on its own. The method relies on connecting dangling bonds at the edges of the two carbon nanostructures, employing the use of two different types of auxiliary structures on a case-by-case basis. The code is implemented in Python 3.7 and generates an output file in the .pdb format containing all the system's coordinates. Acknowledgment: This work was supported by a grant of the Executive Agency for Higher Education, Research, Development and innovation funding (UEFISCDI), project number PN-III-P1-1.1-TE-2016-24-2, contract TE 122/2018.

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