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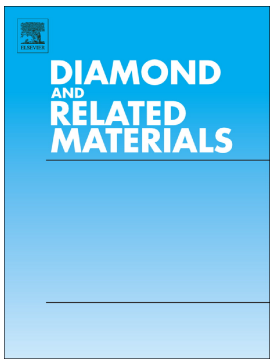

Exceptional ring topology makes diamond allotropes as light-weight superhard materials

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Exceptional ring topology makes diamond allotropes as light-weight superhard materials

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Abstract: Ring topology (RT) is defined as minimal closed rings to characterize the connection features of given atoms so that RT can identify beyond the nearest neighbors the structures of allotropes bearing the same local bonding features, e.g. four-fold coordination in diamond-related materials. Two diamond allotropes with less common 5-8 membered ring topologies were studied by the first-principles calculations in this work. These orthorhombic carbon structures, denoted as L-PHOD and Z-PHOD carbons, respectively, are three dimensional networks connected solely via sp^3 hybridized C-C bonds but their atoms are arranged in a non-hexagonal ring topology different from the conventional diamond. They can be constructed by superimposing Octagon-Pentagon Graphene monolayer consisting of (5-8)-membered

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