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Theoretical investigation on the geometrical symmetry and electronic behavior of the three lower members of diamondoids by using first-principles calculations

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First-principles calculations have been investigated on the geometrical and electronic properties of the three lower diamondoid structures including adamantane ($C_{10}H_{16}$), diamantane ($C_{14}H_{20}$) and triamantane ($C_{18}H_{24}$) molecules. The energy gap obtained from the difference between the highest occupied (HOMO) and lowest occupied (LUMO) molecular orbital for all three structures decreased with the size of diamondoids increasing. The $C_{10}H_{16}$ molecule is the most wide band gap (7.22 eV) and that of $C_{14}H_{20}$ and $C_{18}H_{24}$ are 6.84 eV and 6.59 eV, respectively. The geometry calculations indicated that the geometrical symmetry of three molecular structures appears to be the Td (tetrahedral), D3d (Dihedral) and C2v (Cyclic) point groups for $C_{10}H_{16}$, $C_{14}H_{20}$ and $C_{18}H_{24}$, respectively, which implies the high-symmetry structure for the three lower diamondoids.

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