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Opto-Electronic Properties of Novel Structures: Sila-Fulleranes

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Abstract : Density-functional theory (DFT) was applied to investigate the geometry and electronic properties H-terminated Si-fullerene (Si-fullerane). Natural bond orbital (NBO) analysis confirms sp3 hybridization nature of Si-Si bonds in Si-fulleranes. Quantum confinement effect (QCE) does not affect band gap (BG) so strongly in the size between 1 to 1.7 nm. In contrast, the geometry and symmetry of the cage have significant influence on BG. In contrast to their carbon analogues, pentagon rings increase the stability of the cages. Functionalized Si-cages are stable and can be chemically very active. The electronic properties are highly sensitive to the surface chemistry via functionalization with different chemical groups. As a result, BGs and chemical activities of these cages can be drastically tuned through the chemistry of the surface.

Keywords : density functional theory, sila-fullerens, NBO analysis, opto-electronic properties
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