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Formation of SiC Clusters with Bucky Diamond Structures[1] M. YU, C. GHOSH, C.S. JAYANTHI, S.Y. WU, University of Louisville — SiC clusters with bucky diamond structures have been found in a quantum-mechanical molecular dynamics study based on our recently developed self-consistent and environment dependent Hamiltonian in the framework of a linear combination of atomic orbitals [1]. Starting from a spherically truncated bulk diamond structure, stable structures of SiC clusters containing 147 atoms were studied for various compositions of Si and C atoms. In particular, the following initial configurations were considered: (i) C-rich configuration with Si-core, (ii) Si-rich configuration with C-core, and (iii) an almost equal admixture Si and C atoms. It is found that in the first case Si atoms are dragged to the exterior and a cage-like structure formed, while in the second case some C atoms remain in the interior region and some move to the exterior region forming distorted tetrahedral structures with Si atoms. Finally, in the third case, the bucky-diamond structure is obtained, where the interior has a diamond-like structure and the exterior a fullerene-like structure. The reason why $(SiC)_{147}$ clusters form different stable structures can be understood based on hybridization characteristics of Si (sp^3) and C atoms (sp^1, sp^2, and sp^3), respectively. [1] Leahy *et al.* Phys. Rev. B74, 155408 (2006).

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