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Temperature-dependent properties of SiC Clusters[1] C. GHOSH, M. YU, S. SHEN, C.S. JAYANTHI, S.Y. WU, University of Louisville — Using a semi-empirical quantum mechanics based molecular dynamics simulation [Phys. Rev. B, 74, 155408 (2006)], Si_nC_m clusters were shown to exhibit several types stable structures corresponding to different compositions and distributions of Si and C but a fixed total number of atoms [Ming Yu et al. – APS March 2007]. Specifically, it was shown that an almost uniform admixture of Si and C atoms in a 147-atom SiC cluster exhibited a bucky diamond structure, while the Si-rich and the C-rich stable structures for the same fixed number of total atoms (n+m= 147) exhibited totally different structures with different co-ordinations, bonding, etc. In the present work, we will investigate how equilibrium structures of these different structures evolve with the increase of the temperature from 0K to the melting temperature, and quantities such as pair-distribution functions, electronic density of states, etc. will be calculated up to the melting temperature. This study will provide characterizations of both ordered and disordered SiC clusters, as well as SiC "liquids" in reduced dimensions.

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