Abstract Submitted
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A comprehensive molecular dynamics study on the self-assembly and properties of SiC based cage structures[1] CONGYAN ZHANG, University of Louisville, ZIHUA XIN, Shanghai University, MING YU, C.S. JAYANTHI, S.Y. WU, University of Louisville, SHANGHAI UNIVERSITY COLLABORATION — A molecular dynamics study to investigate a plausible way of fabricating SiC based cage structures has been performed. In this work, the existence of the stable SiC based cage nanostructures SimCn with the size up to about 2.05nm in diameter and the compositions n/(n+m) from 0.4 to 0.6 has been demonstrated using an efficient semi-empirical Hamiltonian method (SCED-LCAO) [PRB 74, 15540 (2006)]. The structural properties are analyzed in terms of the composition, the bonding nature, the surface environment, the local strain, and types of ring structures. It is found that the sp^2 bonding nature between Si and C atoms and the environmental mediation are two key factors for the self-assembly of the stable SiC based cage structures. In particular, the transition from one stable cage structure to another of similar composition might occur due to the mending process in the self-assembly.

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