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Electronic Structure Studies of Silicon Carbide Anionic Nanoclusters PRACHI PRADHAN, ASOK K. RAY, The University of Texas at Arlington — As a continuation of our studies on the high stabilities and electronic structure properties of $Si_8C_2$to $Si_{14}C_2$ clusters and $Si_{60}C_n$(n=3-6) clusters,[1] we report here *ab initio* studies of small $Si_mC_n^-$(1$\leq$ m, n $\leq$ 4) anionic clusters. The theoretical formalism used is the local density approximation (LDA) to density functional theory (DFT) and the *Gaussian03* suite of programs[2] with an all electron 6-311++G** basis set has been used. Complete geometry optimizations of different possible structures have been carried out. Carbon-rich and silicon rich species show distinctly different patterns with respect to the vertical detachment energies. For carbon-rich aggregates, the VDE's show an even odd alternation, similar to that of the carbon anions. We present results on binding energies, relative energies, fragmentation energies, vertical detachment energies, vibrational frequencies, and adiabatic electron affinities[3] for the optimized clusters. Detailed comparisons with published data in the literature will also be presented. * Work supported, in part, by the Welch Foundation, Houston, Texas (Grant No. Y-1525). [1]M. N. Huda and A. K. Ray, Phys. Rev. A (R) **69**, 011201 (2004); Eur. Phys. J. D **31**, 63 (2004). [2] *Gaussian03*, Revision A.1, M. J. Frisch *et al.,* Gaussian Inc., Pittsburgh, PA , 2003. [3]P. Pradhan and A. K. Ray, J. Mol. Structure (Theochem), in press.

Prachi Pradhan

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