

Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Electronic Structure Studies of Silicon Carbide Cationic Nanoclusters PRACHI PRADHAN, ASOK K. RAY, The University of Texas at Arlington — As a continuation of our studies on the high stabilities and associated electronic structure properties of Si_8C_2 to Si_{14}C_2 and Si_{20}C_n ($n=3-6$) clusters,¹ we report here detailed *ab initio* electronic and geometric structure studies of small Si_mC_n^+ ($1 \leq m, n \leq 4$) cationic clusters. The theoretical formalism used is the local density approximation (LDA) to density functional theory (DFT) and the *Gaussian03* suite of programs² with an all electron 6-311++G** basis set has been used. Complete geometry optimizations of different possible structures have been carried out. The stability of the clusters varies with the ratio of the number of silicon to carbon atoms in the cluster. In contrast to the neutral clusters,³ cationic clusters appear to prefer more open structures. Results will be presented for binding energies, relative energies, fragmentation energies, vibrational frequencies, and adiabatic ionization potentials³ 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) ¹M. 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. ³P. Pradhan and A. K. Ray, J. Mol. Structure (Theochem), in press.

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Date submitted: 29 Nov 2004

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