Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Single and Multiple Rings, and Cages in SiO_x Clusters PENEE CLAYBORNE, ARTHUR REBER, J. ULISES REVELES, SHIV KHANNA, Department of Physics, Virginia Commonwealth University, Richmond Va, 23284, A. WELFORD CASTLEMAN, Department of Chemistry and Physics, The Penn State University, University Park, Pa 16802 , ASHRAF ALI, Laboratory for Extraterrestrial Physics, Code 691 NASA Goddard Space Flight Center, Greenbelt Md, 20771
— Theoretical studies on the geometry, electronic structure and stability of Si_nO_m clusters have been carried out within a gradient corrected density functional formalism. It is shown that the ground states of small Si_nO_n clusters containing upto 4 units are single rings. The first Si-Si bond appears at Si_5O_5, and starting at this size, the elementary rings begin to assemble into multiple rings that eventually lead to cages. The ground state structures at larger sizes have a central core of pure Si atoms decorated by outer shell of SiO units. An analysis of the fragmentation patterns shows that Si_7O_7 and $Si_{10}O_{10}$ are particularly stable species. The results of our investigations on the Si_nO_{n-1} and Si_nO_{n+1} species will also be presented. In particular, we will examine possible reaction mechanisms that could lead to the formation of SiO_2 from SiO molecules in interstellar space.

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Date submitted: 28 Nov 2005 Electronic form version 1.4