

Abstract Submitted
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Structure, Growth and Optical Properties of Si_nO_m Nanoparticles: From SiO molecules to Silicates in Circumstellar Space¹ SELVARENGAN PARANTHAMAN, ARTHUR REBER, PENECE CLAYBORNE, SHIV KHANNA, Virginia Commonwealth University, A. WELFORD CASTLEMAN JR., Pennsylvania State University — Synergistic effort combining formation of clusters in molecular beams and first principles electronic structure studies within a gradient corrected density functional scheme are employed to examine the geometries, stability, vibrational frequencies and optical properties of Si_nO_m clusters. It is proposed that the oxygen enrichment needed to form silicates in interstellar space, starting from SiO molecules can occur via two processes. (1) Chemically driven compositional separation in $(\text{SiO})_n$ motifs resulting in oxygen rich and oxygen poor regions, and (2) reaction between Si_nO_m clusters leading to oxygen richer and poorer fragments. Theoretically calculated optical and infrared spectra of Si_nO_m clusters exhibit features observed in the extended red emissions and blue luminescence from interstellar medium indicating that the Si_nO_m fragments could be contributing to these spectra.

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