

Abstract

The purpose of this poster is to present some of the results obtained in the course of a study of the reactions involving atomic Carbon and Silicon in their 3P and 1D atomic states and singlet silane molecule. These reactions are of interest given their relevance to the mechanisms involved in preparation of semi-conducting (under extreme conditions), micromechanically desirable silicon carbide (SiC) thin films, as well as to those of photochemical reactions inside interstellar/circumstellar dust (composed of small carbon- and silicon-containing meta-stable molecules, radicals) which have been found to contain silane (and methane). The primary results of energetics calculations include previously unknown van der Waal intermediates, suggesting that the insertion intermediates reported in previous studies are accessible through these vdW complexes, and the master equations derived to study the chemical kinetics of these systems must take them into account for better reaction rate estimates.

Acknowledgements: Above investigation has been possible due to the support of HASI.