

Adsorption Energies of Molecules and Molecular Fragments on Si(100)

The adsorption of a number of molecules on Si(100) have been actively studied in recent years due to their importance in chemical vapor deposition (CVD) processes for microelectronics, optoelectronics and optical device fabrication. Yet the energetics of the adsorbed species produced are generally not available, since they dissociate before desorbing and/or desorb as some silane adduct rather than as the pure adsorbate. Techniques such as temperature programmed desorption or equilibrium adsorption isotherms have been used to get adsorption energetics on Si(100), but these techniques only work for the few species whose adsorption is totally reversible. If any dissociation occurs or if the species converts into a different structure upon heating before desorption, then these techniques fail to provide the adsorption energy of interest. As shown in our Prior Results, we now have the capability to *directly* measure adsorption energies on Si(100), although at the present time only with metal atom beam. With the additional molecular beam mentioned above, we will be able to study molecular gases as well.

We propose to demonstrate the ability to study CVD-related processes on Si(100) using molecular gases. Initially, we will study the adsorption of TiCl_4 , Si_2Cl_6 and cyclopentene. The adsorption of TiCl_4 and Si_2Cl_6 will provide intermediates of interest in growing CVD Ti, TiN and Si films, and in Si etching. Cyclopentene adsorbs to produce the [2+2] Diels-Alder adduct, so that its adsorption energy should provide the strength of a covalent C-Si bond between an adsorbate and the Si(100) surface. This energy is of interest both in CVD processes and in understanding a variety of recently-developed approaches for organofunctionalization of Si surfaces with applications in sensors and microfluidics fabrication.