

Potential Energy Calculations for Water Adsorption on Poly (methyl methacrylate)

Mateusz J. Zuba, P. Howard, B. Familo, T. Kane, R. Netusil, and C. C. Ilie

The generosity of the NOYCE Research Grant enabled me to focus on the study of various polymers. The main goal was to study the molecular orbitals of poly (methyl methacrylate) (PMMA) and calculate the energy band gap. We obtained the activation energy from thermal desorption spectra of water on poly (methyl methacrylate) by employing Arrhenius analysis. Thermal desorption of PMMA is coverage independent with peaks at the same temperature. Activation energy of desorption may increase with increasing water coverage, i.e. the amount of water exposed to the system. We also performed the potential energy calculations for our system: two polymer chains and water molecules. The method by which potential energy calculations were performed involved HyperChem Professional 8.0; a very sophisticated molecular modeling software known for its quality, flexibility, and ease of use. As seen using HyperChem water molecules take a favorable position above the PMMA chains. Double bonded oxygen atoms of PMMA favor the Hydrogen atoms of the water molecule. CH₃ ligands tend to turn the oxygen of water down towards the polymer backbone. Potential energy plots (in eV) for the water molecule as a function of distance from PMMA chains along the lateral to the backbone chain were obtained. These calculations were used in scientific papers.