Theoretical Characterization of Low-energy Particle Deposition on PMMA Surfaces.

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The chemical processes that lead to polymer surface modification via low energy particle deposition were analyzed using molecular dynamics simulations (MD) and first principles calculations. The MD simulations performed used the reactive empirical bond order (REBO) potential to identify key products as a result of the interaction between the deposited particles and the surface of the polymer chains. A variety of particles (H^+, C_2H^+, C_2F^+, $CH_2^{+/\cdot}$ etc.) were deposited on the poly(methyl methacrylate) (PMMA) surface and, a large number of likely products were identified from the MD simulations, which did not treat the charging explicitly. The reaction mechanisms to obtain the identified products were subsequently examined using Density Functional Theory (DFT) methods. The structures of the reaction species and energy barriers were determined using the B3LYP hybrid functional and subsequent CCSD (Coupled Cluster Singles and Doubles) calculations were performed on each optimized structure to obtain more accurate energetics. The calculations provided key information about the mechanism of surface reactions and will be incorporated into further development of many-body reactive potentials. This work is supported by the National Science Foundation grant number CHE 0809376.