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Conformational Impact on Amino Acid-Surface π-π Interactions on a (7,7) Single-Walled Carbon Nanotube: A Molecular Mechanics Approach LINDA GRABILL, ANDREAS RIEMANN, Western Washington University — A study of π-π interactions between a (7,7) single-walled carbon nanotube (SWNT) and three different aromatic amino acids (AAA), namely L-tyrosine (Tyr), Ltryptophan (Trp), and L-phenylalanine (Phe) was conducted with a molecular mechanics (MM) approach. For each of the amino acids we investigated the behavior of six different conformers. We examined the impact of the so-called edge effects by testing the parameters of the built-in switching function in MM. We found the optimal SWNT length to be approximately 80 angstroms for the size of the molecules in our conformational studies. The positional effect of electron withdrawing groups with respect to the aromatic tail was studied to understand the influence of this interaction specific to adsorption strength and geometry. We decomposed the aromatic amino acid−surface interactions into three components: overall energy, aromatic ring, and amino acid head adsorption energies. We found that the ability of the amino acid's head to interact with the surface π-densities had a greater impact on the overall energy than the amino acid head interaction with its substituent's aromatic ring's π-electrons.

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