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Computer Modeling of the Self Assembly of Tyrosine LINDA GRABILL, Western Washington University, ERIC KREBS, Oregon State University, ANDREAS RIEMANN, Western Washington University — We used Scanning Tunneling Microscopy (STM) results to obtain information on bond symmetry, spacing, and general orientation of amino acids adsorbed on a graphite surface. One goal of our research is to compliment these experimental results using two computer programs , Igor and HyperChem, to model energetic behaviors between two molecules. This computational approach is used for a better understanding of the geometry and binding of the amino acid molecules. Previously, computer modeling and STM scans on Methionine, a neutral and non-polar amino acid with a Sulfide functional group, resulted in good agreements between experiment and modeling. These results were promising and led us to attempt the same for Tyrosine, a neutral and polar amino acid with a hydroxyphenyl functional group. Our STM results for Tyrosine showed a monolayer film with Tyrosine molecules ordered in parallel rows angled alternating at 110 degrees. For this configuration our approach to modeling was modified from that of Methionine. We have run computer simulations with HyperChem using the Amber94 force field, modeling the molecules in their neutral and zwitterionic states and using a single sheet of graphite as the substrate. I will be presenting first results of these calculations.

Linda Grabill
Western Washington University

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