135d Organic Functionalization of Semiconductors Using Amino Acids; Quantum Resonance Coupling

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We have used DFT to simulate the attachment of amino acids and various unique organic molecules to the Si(100)-2x1 surface. These structures have potential applications in molecular electronics and sensors if their structures can be controlled and if the resulting interface electronic structure provides appropriate electronic transport properties. We will present a summary of the various unique reactions of amino acids on Si(100)-2x1 and focus on certain organics functionalities that are stabilized on Si and Ge by quantum mechanical resonance which stabilizes the product and leads to stronger electronic coupling between the attached organic and the semiconductor substrate which might be useful in improving electrode-molecule charge transfer for organic-semiconductor molecular electronic devices. We will also discuss the accurate simulation of the electronic band structure of these molecular junctions required for correct prediction of the electron transport across these junctions. We have found that the common DFT methods are inadequate for this task, although the KMLYP method correctly predicts the HOMO and time-dependent KMLYP (TD-KMLYP) correctly predicts the LUMO energy.