DFT Study of Amino Acids on Si Surface for Hybrid Organic-Semiconductor and Protein-Semiconductor Structures GUILLUM-AME DUPONT, CHARLES MUSGRAVE, Stanford University — We have used DFT to investigate the formation of hybrid organic- inorganic interfaces between amino acids and silicon surfaces. Not only do amino acids provide a large library of novel organic attachment chemistries to semiconductors, but the reactivity of their side chains also serve as models for the local interactions involved in forming protein-semiconductor interfaces. The amino acid common group is found to react through several low energy pathways, with OH dissociation of the carboxyl group being the most kinetically favorable. Consequently, reaction of amino acids through the amine and carboxyl functionalities is not expected to be selective. The reactivity of many of the amino acids are similar to those of their simpler organic analogues, although we have found several cases which display unique, and possibly useful properties not exhibited by organic functionalities previously considered. Of special interest are attachments of particular amino acid side chains which create quantum mechanical resonances between the amino acid and the semiconductor substrate that may find application in molecular electronics.