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Theoretical investigation of the atomic and electronic structure of amino acids on Si(100) surfaces XUAN LUO, GEFEI QIAN, CELESTE SAGUI, CHRISTOPHER ROLAND, Department of Physics, NCSU — There are currently considerable efforts underway to combine silicon-based device technology with myriad of organic molecules, thereby fabricating new structures that take advantage of the tunable electronic and optical properties of organic molecules. A key aspect of this integration process is binding of the organics to the silicon surfaces. As part of this effort, we have been investigating the binding of several amino acids – the building blocks for proteins – on the Si (100) surface with state-of-the art density functional theory methods. Specifically, the binding between the buckled Si(100) and the NH2, CH2, COOH, C=0 and NC entities at various surface sites have been investigated. We report and discuss on the resulting structures and their electronic properties.

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