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Biotin chemisorption on clean and hydroxylated Si-SiC(001) surfaces YOSUKE KANAI, Princeton University, Princeton, NJ, GIANCARLO CICERO, GIULIA GALLI, LLNL, Livermore CA, ANNABELLA SELLONI, ROBERTO CAR, Princeton University, Princeton, NJ — In recent years, there have been substantial experimental efforts toward achieving nanoscale functionalization of semiconductor surfaces. One of the main motivations of such experiments is biosensing application. Biotin is a leading candidate for such functionalization because of its strong, unmatched affinity to specific proteins such as Streptavidin. On the other hand, silicon carbide (SiC) has emerged as a promising biocompatible material that may be employed in new biomedical devices. Using Density Functional Theory, we have carried out a theoretical investigation of the structural and electronic properties of biotin after chemisorption on both the clean and hydroxylated Si-SiC(001). We find that, upon chemisorption, Biotin retains the electronic properties responsible for its strong affinity to proteins. While the electronic states of the hydroxylated surface undergo negligible changes in the presence of biotin, those of the clean surface are substantially affected by the presence of the molecule. This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

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