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Structure and adsorption mechanisms of thiol self-assembled monolayers on GaAs (001) surfaces OLEKSANDR VOZNYI, JAN J. DUBOWSKI, University of Sherbrooke — Self-assembly of organic molecules on solid substrates attracts a lot of interest from both fundamental and practical perspectives. Particularly, alkanethiol SAMs on GaAs surfaces can be used, e.g., for surface passivation, bio- and chemical sensing, molecular electronics and nanolithography. However, the progress of the investigation of this material system is hindered by problems of reproducibility of SAMs growth due to insufficient understanding of the deposition process on the atomic level and a lack of experimental characterization techniques. In this work, we present the results of ab initio modeling of thiol SAMs on GaAs (001) surface which helps to resolve the SAM structure, chemistry of bonding to substrate, adsorption kinetics and energetics. We also compare the GaAs case to a prototypical system of thiols on Au and discuss differences the semiconductor surface brings to the process.

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