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Theory of nanostructures for sensing applications

Karl Sohlberg
Department of Chemistry, Drexel University, USA

In this talk I will present a computational procedure for predicting hole mobility in a thin-film molecular solid in the presence of an adsorbate. The procedure starts by describing the effect of surface defects on mobility. These defects may take the form of vacancies in the surface layer of the film or molecules adsorbed onto the surface of the film. By treating adsorbed molecules as defects it is possible to derive a relationship between the fractional coverage of an adsorbate and mobility in the film using a method based on an implementation of Marcus hop rate theory. Application of the Langmuir adsorption model then yields a relationship between analyte partial pressure and mobility in the film. Using this theory we study the potential of several organic molecular solids for sensing applications. We have characterized simple oligoacene species, (especially naphthalene and pentacene) and for validation, the unrelated species α,ω dihexylquaterthiophene (DH4T). Results are consistent with published studies of the relationship between mobility and defect density in semiconductors and yield insight into the electronic structure characteristics that render a material suitable for use as a probe of the presence of an adsorbate. The theory is used to understand the selective response of Ellagic acid nanostructures to the presence of nitrobenzene.

Biography

Karl Sohlberg is an Associate Professor of Chemistry at Drexel University, (Philadelphia, PA). His broad research area is theoretical and computational materials chemistry, with specific research programs in molecular nano-devices and complex catalytic materials. Before joining the Drexel faculty in 2000 he was an Oak Ridge Associated Universities postdoctoral fellow at Oak Ridge National Lab. Earlier, he held postdoctoral appointments at The Johns Hopkins University and Brigham Young University. He received his PhD in physical chemistry from the University of Delaware. At Drexel he teaches "Math and Computer Skills for Chemists" and "Computational Methods of Modeling Molecules". He also serves as an Associate Editor of the *Journal of Computational and Theoretical Nanoscience.*

kws24@drexel.edu