Abstract Submitted
for the MAS14 Meeting of
The American Physical Society

Control of the interfacial chemical coupling between organic adsorbates and semiconductor surfaces revealed with Raman spectroscopy[1]

FLOYD HILTY, Bowling Green State University, ANDREW KUHLMAN, University of Konstanz, ALEXEY ZAYAK, Bowling Green State University — In the search for methods of studying chemical properties of surfaces and heterogeneous interfaces we focus on Raman scattering, aiming to reveal physical and chemical processes that vary on the scale of a few chemical bonds, with information not only about a particular chemical species, but also about its immediate chemical environment. While the so-called "chemical enhancement" on metallic surfaces has been previously investigated in the context of SERS, in this work we use first-principles calculations to reveal general trends of the chemical modification of Raman spectra of organic species after being chemically absorbed on semiconductor surfaces. We examine the binding of a trans-1,2-two(4-pyridyl) ethylene molecule to various crystallographic facets of a PbSe, showing that Raman spectra of adsorbed species vary significantly on different crystallographic facets of PbSe, which is correlated with the electronic structure of each type of semiconductor surface. Based on that picture, we demonstrate the possibility of tuning the interfacial coupling by applying an external electric potential, achieving not only chemical tunability of the interface, but also a direct method of studying surface chemistry with Raman.

[1] We acknowledge "Building strength" grant from BGSU and XSEDE project TG-DMR130080.

Alexey Zayak
Bowling Green State University

Date submitted: 25 Aug 2014 Electronic form version 1.4