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Raman spectroscopy of electric-field-tuned molecule-semiconductor interface[1] ALEXEY ZAYAK, FLOYD HILTY, ANDREW KUHLMAN, Bowling Green State University — In the search for methods of studying chemical properties of surfaces and atomic-scale heterogeneous interfaces, Raman scattering promises significant potential for measuring physical and chemical properties that vary on the scale of a few chemical bonds, reporting not only about a particular chemical species, but also about the immediate chemical environment. In this work we use first-principles (DFT) computations to investigate 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 the PbSe semiconductor surface and show that we can tune the degree of the interfacial chemical coupling by means of an external electric field, and at the same time, observe the induced changes in Raman spectra. In the process of applying electric bias, we observed a crossover between two regimes of the interfacial electron-vibron coupling: with vibration-induced charge transfer; and without it.

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