

Abstract Submitted
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Understanding Metal-Adsorbate Binding with Surface-Enhanced Raman Spectroscopy: Theory and Experiment¹ ALEXEY ZAYAK, Molecular Foundry, LBNL, HYUCK CHOO, EECS, UC Berkeley, YING HU, Bioengineering Dpt., Rice University, JEFFREY BOKOR, EECS, UC Berkeley, STEFANO CABRINI, JAMES SCHUCK, JEFFREY NEATON, Molecular Foundry, LBNL — Building on recent work [1], we use a combination of density functional theory (DFT) calculations and surface-enhanced Raman spectroscopy (SERS) measurements to explain experimentally observed variations in SERS data of an organic molecule, trans-1,2-bis(4-pyridyl) ethylene (BPE). For the BPE on Au surfaces, our DFT calculations provide a quantitative description of chemical enhancement (CE), and elucidate that variations reported in experiments arise from a convolution of two factors: a nonuniform frequency dependent electromagnetic enhancement, and dependence of CE on the sample incubation time. The later reveals aspects of the binding kinetics of BPE to Au surfaces.

[1] A. T. Zayak, et. al., arXiv:1011.1873v1

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