Med Chem (Los Angeles) 2018, Volume 8
DOI: 10.4172/2161-0444-C2-043

18th International Conference on

Pure and Applied Chemistry

August 31- September 01, 2018 | Toronto, Canada

By Indirections find directions out: Utilizing SERS to deduce molecular structure at metallic surfaces

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Surface-enhanced Raman spectroscopy (SERS) probes the adsorbates at the plasmonic substrate and offers high sensitivity with molecular identification capabilities. In this study, we present a refined methodology concerning the supporting substrate in the computation of the Raman spectra. The supporting substrate is taken into account by employing a periodic slab model when doing the geometry optimization and normal mode analysis. We find that the interaction with the surface induces internal distortion in the molecule. The distortion leads to spectral shifts in the computed Raman spectrum. By comparing a low-temperature surface-enhanced Raman spectroscopy (LT-SERS) experiment of rhodamine 6G (R6G) with the computed Raman spectra for a series of adsorption geometries, we found that the binding state captured in the experiment tends to possess the least internal distortion. In this way, we demonstrate that using computations, we can deduce the molecular structure and geometry of the molecule.

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