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Raman spectra of benzene derivatives adsorbed on metal substrates D.A. ALEXSON, S.C. BADESCU, O.J. GLEMBOCKI, S.M. PROKES, R.W. RENDELL, U.S. Naval Research Laboratory — We study the molecular orientations of several benzene derivatives on large Ag and Au clusters via first-principles calculations. We find the lowest-energy structures, several local minima and the diffusion barriers for benzene, nitrobenzene, 2,4-dinitrotoluene (DNT) and 1,4-benzenedimethanethiol (BDMT). The theoretical calculations are compared to experimental measurements of SERS for 2,4-DNT and 1,4-BDMT on Ag and Au coated dielectric nanowires.

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