ABNORMAL RAMAN BANDS OF AROMATICAL AMINES AND BENZYL RADICALS ADSORBED ON METAL SURFACES

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In the work we present our recent works focusing on the chemical enhancement effect of Raman cross section of the wagging vibrations in aromatic amines and benzyl radical adsorbed on metal surfaces. These molecules can display giant chemical enhancement effect in Raman intensity of the specific wagging vibrational modes. To understand the origin of the Raman intensity enhancement, we calculated the potential energy surfaces along the vibrational mode and analysed the change of polarizability due to the binding interaction. Our results also showed that the change of the polarizability derivatives is closely associated with the binding interaction and the orbital hybridization. Furthermore, we also analysed the anharmonicity of the potential energy surface and the vibrational coupling effect of the wagging vibration contributing to the Raman intensity. The Raman features of these special vibrational modes significantly change in vibrational frequency and the relative Raman signal. Finally, we further predict the contribution of the charge transfer state to the relative Raman intensity based on the density functional theoretical calculations.