

## Raman spectroscopy of the PTCDA–inorganic semiconductor interface: evidence for charge transfer

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### Abstract

In the present work, we investigate the vibrational properties of a PTCDA molecule with an additional positive or negative charge using density functional theory. With respect to the calculated vibrational frequencies of the neutral molecule, some modes in particular in the region 1200–1800 cm<sup>-1</sup> show large shifts. These calculations are compared with resonant Raman spectra of sub-monolayer PTCDA films on passivated semiconductor surfaces, both before and after annealing the deposited films at elevated temperatures (350 °C). Independent of the sample treatment, the sub-monolayer Raman spectra correspond quite well to reference spectra obtained for thicker films, and we find no evidence for the strong shifts predicted in the calculations for the charged species. From the small changes in the mode frequencies it can be concluded that any charge transfer present involves significantly less than one elementary charge.

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