

Valence shell photoelectron spectroscopy for PAHs and its significance

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Polycyclic aromatic hydrocarbons (PAHs) are efficient absorber of UV and fluoresce in IR giving rise to unidentified interstellar bands (UIB) observed in stellar medium [1]. Hence to study the stability/energy dissipation mechanism of PAHs under harsh interstellar environment and relate various excitation modes to the UIBs, the state selective photoelectron spectrum (PES) measurements were done on pyrene and fluorene using synchrotron radiation source facility at Elettra for 15 to 40 eV photon beam. The PES of a molecule is typically associated with a broadening due to Franck-Condon (FC) overlap of vibrational states. Using Hartree-Fock (HF) and Density functional technique (DFT), the FC factor for vibrational progression in $D_0 \leftarrow S_0$ transition are calculated within harmonic approximation which compares well with our experimental results. The C-C trans-annular stretching in plane mode with ag symmetry is found to be the dominant mode of vibration corresponding to $\sim 1400 \text{ cm}^{-1}$ band for all PAHs and is attributed to one of the prominent feature observed in UIR bands of ISM [2]. Such calculations would be very useful in determining the IR fluorescence processes in ISM where UV photo ionization is a very common process. The PES as a function of photon energy showed a sharp increase in inner valence photoelectron cross section (binding energy 10-12 eV) for around 16-25eV photon energy due to plasmon excitation (Fig. 1). Outer valence Green's function technique is used to assign the symmetry and binding energy to molecular orbital [3].

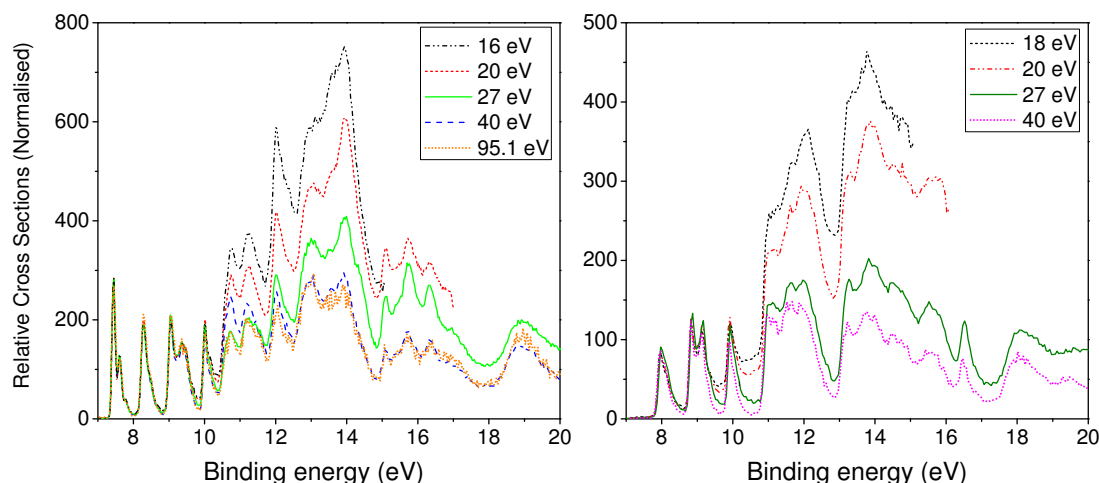


Figure 1: Pyrene (left) and fluorene (right) photoelectron spectra for different photon energy.

References

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