Resonances in molecules and molecular clusters

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Temporary anion states (also known as resonances) can enhance most electron-induced processes. More interestingly, they can be chemistry initiators by leading to the break-up of the molecule into at least one reactive species. Resonances are also important in other molecular processes, for example, photodetachment and associative detachment. Theoretical research on their identification and characterization is therefore an active area particularly, but not uniquely, associated to the understanding of electron-induced process in biological systems.

Scattering methods are able to accurately describe resonances: the modelling of shape resonances can be done using several scattering approaches, both for small and larger molecules. Core-excited resonances are harder to model accurately. However, both types of resonances (and vibrational Feshbach resonances) play an important role in biological radiation induced damage and electron transfer reactions. Recent joint theoretical and experimental work on pyrimidine [1] and thiophene [2] (see Figure 1) using the R-matrix method [3] and electron energy loss spectroscopy has confirmed the ability of theory to accurately describe core-excited resonances in biologically relevant molecules.

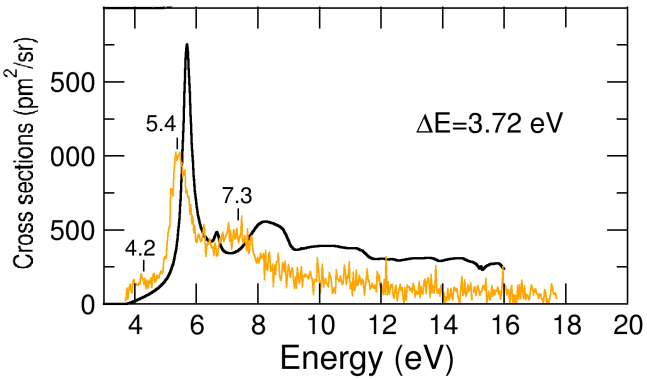

Figure 1: Calculated (smooth line) and measured (jagged line) excitation function for electron-thiopene collisions for energy loss ΔE=3.72 eV corresponding to excitation into the first singlet electronic state. The electron scattering angle is 90°. The peaks corresponding to the three visible resonances are indicated. Results published in [2].

Nonetheless, electron scattering process don't always take place in the gas phase where the target molecule is isolated from others. In biological environments, for example, relevant molecules are surrounded by water. In order to bridge the gap between the pure gas phase and the actual environment where many collisions occur, molecular clusters are being investigated [4]. Using the R-matrix approach, calculations of electron scattering from pyridine/thymine-$(H_2O)_n$ for n=1,2,3,5 have been performed and the different effects of microhydration analyzed. The results have been linked to experiments on microsolvated uracil and thymine.

[1] Regeta K, Allan M, Mašín Z and Gorfinkiel J D 2016 *J. Chem. Phys.* **144** 024302
[2] Loupas A, Regeta K, Allan M and Gorfinkiel J D 2018 *J. Phys. Chem.* A **122** 1146
[3] Tennyson J 2010 *Phys. Rep.* **491** 29
[4] Gorfinkiel J D and Ptasinska S 2017 *J. Phys B.* **50** 182001