INVESTIGATING ELECTRONIC PROPERTIES OF IONIZED PAH CLUSTERS

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Polycyclic aromatic hydrocarbon (PAH) clusters have been proposed as candidates for evaporating very small grains that are revealed by their mid-IR emission at the surface of UV-irradiated clouds in interstellar space[a]. This motivates studies on the photostability and spectroscopic signatures of such species to validate their presence in interstellar environments and constrain their survival therein. We have used the molecular beam chamber SAPHIRS and the photoelectron-photoion coincidence spectrometer DELICIOUS II[b] at the SOLEIL synchrotron facility to characterize the electronic properties of cationic coronene ($C_{24}H_{12}$) clusters up to the pentamer. These experimental results are analysed in the light of electronic structure calculations[c]. In particular a Density Functional Tight Binding + Configuration Interaction scheme[d] is developed to describe charge delocalization in these large systems and calculate the ionization potential, vibrational spectra, and charge transfer excited states. For the coronene dimer cation, complementary measurements are performed with the PIRENEA set-up to quantify some of the electronic transitions, in particular their oscillator strengths that cannot be extracted from the photoelectron spectroscopy. Emphasis will be put on the evolution of the spectra with cluster size.

[a] M. Rapacioli, C. Joblin and P. Boissel *Astron. & Astrophys.* **429** (2005), 193-204.
[b] G. Garcia, H. Soldi-Lose and L. Nahon *Rev. Sci. Instrum.* **80** (2009), 023102.
[c] Joint ANR project GASPARIM, ANR-10-BLAN-501
[d] M. Rapacioli, A. Simon, L. Dontot and F. Spiegelman *Phys. Status Solidi B* **249** (2) (2012), 245-258.