

## Structure and energetics of PAH clusters of interstellar relevance

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Polycyclic aromatic hydrocarbons (PAHs) are key species in the physics and chemistry of UV-irradiated astronomical environments [1]. Still, our understanding of the formation and evolution of these species remains very partial and is a challenge for astronomers, physicists and chemists. From the analysis of the mid-infrared spectra, Rapacioli et al. [2] have proposed an evolutionary scenario in which gas-phase PAHs are produced by photo-evaporation of nanograins, which could be PAH clusters.

In the collaborative frame of the ANR project GASPARIM, we are studying the electronic properties and stability of ionized PAH clusters. Charge delocalization in these large systems is described using a density functional tight-binding method combined with an additional valence-bond configuration interaction scheme [3]. Theoretical studies predict that there should be an ionized core of 2-4 units and that larger ionized clusters have evaporation rates for the loss of one monomer that are close to the neutral ones [4].

We have used a molecular beam coupled to the photoelectron-photoion coincidence spectrometer DELICIOUS II/ III [5] at the VUV beamline DESIRS of the synchrotron SOLEIL to characterize the electronic properties of cationic coronene (C<sub>24</sub>H<sub>12</sub>) and pyrene (C<sub>16</sub>H<sub>10</sub>) clusters up to the pentamer and heptamer, respectively. The obtained experimental results are compared with theoretical predictions. We will show that the good match between measured and calculated values for the ionization potential, gives us strong confidence into the predicted structures for these PAH clusters. We will also present first results on the dissociation of the clusters, in particular their appearance energies.

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### References

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**Primary author:** Dr JOBLIN, Christine (Université Toulouse 3/ CNRS, IRAP)

**Co-authors:** Dr BONNAMY, Anthony (Université Toulouse 3 / CNRS, IRAP); Dr GAMBOA, Antonio (Université Paris-Sud 11 / CNRS, ISMO); Dr SIMON, Aude (Université Toulouse 3 / CNRS, LCPQ); Dr FALVO, Cyril (Université Paris-Sud 11 / CNRS, ISMO); Dr KOKKIN, Damian (Université Toulouse 3 / CNRS, IRAP); Dr SPIEGELMAN, Fernand (Université Toulouse 3 / CNRS, LCPQ); Dr GARCIA, Gustavo (Synchrotron SOLEIL); Dr SABBABH, Hassan (Université Toulouse 3 / CNRS, IRAP); Dr NAHON, Laurent (Synchrotron SOLEIL); Dr DONTOT, Léo (Université Toulouse 3 / CNRS, LCPQ); Dr RAPACIOLI, Mathias (Université Toulouse 3 / CNRS, LCPQ); Dr PIRALI, Olivier (Université Paris-Sud 11 / CNRS, ISMO); Prof. PARNEIX, Pascal (Université Paris-Sud 11 / CNRS, ISMO); Prof. BRÉCHIGNAC, Philippe (Université Paris-Sud 11 / CNRS, ISMO); Dr PINO, Thomas (Université Paris-Sud 11 / CNRS, ISMO)

**Presenter:** Dr JOBLIN, Christine (Université Toulouse 3/ CNRS, IRAP)

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