Theoretical studies of $(PAH)_m(H2O)_n^{+/0}$ in Ar matrices : model and benchmark.

C. IFTNER[1], X. KORCHAGINA[1], A. SIMON[1], F. SPIEGELMAN[1]

[1]*Laboratoire de Chimie et Physique Quantique*
Université Paul Sabatier,
Christophe.iftner@irsamc.ups-tlse.fr

Interest regarding Polycyclic Aromatic Hydrocarbons (PAH) systems has grown during the last decades, since the discovery in the mid-eighties of the Aromatic Infrared Bands, a set of mid-IR emission bands that was assigned to a population of PAHs[1]. Despite many experimental and theoretical studies, no specific PAH molecule has been identified yet. Among experimental studies, cryogenic matrix experiments have been performed[2]. To our knowledge, theoretical studies to quantify the influence of the Argon matrix on the IR spectra are scarce[3].

In this poster, we present and benchmark a theoretical approach for the description of $(PAH^{+/0})Ar_n$ clusters. This approach is based on a QM (quantum mechanical)/MM (molecular mechanics) scheme. The QM part is computed with the Density Functional based Tight-Binding DFTB) method in its Self-Consistent Charge (SCC)version[4]. The interaction between $PAH^{+/0}$ and the Ar atoms is determined by adding to the diagonal elements of the SCC-DFTB Hamiltonian a perturbation term ($u_{x\text{-}Ar}$, x refering to an atomic orbital of C or H) obtained from the fits of diatomic C-Ar and H-Ar CCSD(T) potentials. In order to benchmark this approach, we determined the influence of the number of Ar atoms on the ionization potential of benzene, and compared our results to DFT and CCSD(T) data, and also with experimental and theoretical results available in the literature.

The objectives of our future work is to obtain dynamical and spectroscopic properties for $(XPAH^{+/0})Ar_n$ systems ($PAH=C_{24}H_{12}$, $X=H_2O$) in relation with cryogenic matrix experiments, in particular those conducted by J. Mascetti[5]. Our ultimate goal is to improve our understanding of the thermal, dynamical and spectral properties induced by the matrix.

References

[1] A.G.G.M. Tielens, *Annu. Rev. Astron. Astrophys*. **46**, (2008)

[2] F. Salama, C. Joblin and L. J. Allamandola, *Planet. Space Sci.*, **43**, 10 (1995)

[3] F. Calvo , Cyril Falvo, and Pascal Parneix, *J. Chem. Phys.* **138**, 034305 (2013)

[4] M. Elstner, D. Porezag, G. Jungnickel, and all, *Phys. Rev.* B **58**, 7260 (1998).

[5] Zohra Guennoun, Christian Aupetit, and Joëlle Mascetti, *J. Phys. Chem. A* **115**, 10 (2011)