Theoretical insights into the dissociation of PAH clusters

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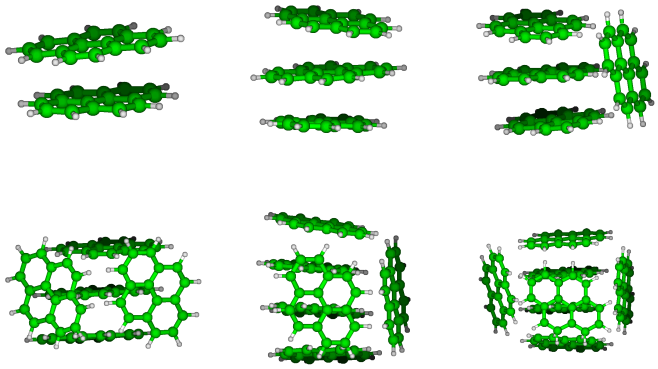
Astrophysical observations suggest that PAH are produced by photoevaporation of very small grains which could be PAH clusters stabilized by van der Waals and electrostatics interactions or by charge resonance between the PAH units in the case of ions. Containing tens to few thousands of atoms, such systems can hardly be approached via traditional ab initio schemes at the moment. Density functional based tight binding method (DFTB, an approximate DFT scheme) allows to deal with systems of this size range. Unfortunately, it inherits from DFT the difficulties to describe the typical interactions met in molecular clusters, in particular charge resonance in ions.



Most stable structures obtained for cationic pyrene clusters

This presentation will give an overview of how DFTB can be modified to become a realistic and efficient tool to investigate the structural, electronic and energetic properties of PAH clusters. We will compare the computed observables with recent experimental results and will use the theoretical electronically excited potential energy surfaces to propose mechanisms involved in photo-dissociation experiments.

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References

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