**Electron Density, the Driving Tool towards Dynamics and Reactivity of Systems ?**

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The fast development of photo-induced and time resolved diffraction leads to fundamental questioning about the proper modelisation of systems out of equilibrium.

Based on the role of Hellmann-Feynman force and its impact onto molecular dynamics, we have modelled the evolution of the charge density of simple molecules along a reaction path. Moreover, we have addressed the change of charge density in a molecular chain undergoing strong distortions, such as those initiating na soft mode transition.

The planned developments are strongly connected with the Cluster Partitioning Model recently developed in our group [1,2] which allows for a description of one particle density matrix of complex systems through a superposition of local contributions taking into account realistic environmental effects.

[1] Ragot S., Gillet J.M., Becker P., *Physical Review*, 2002, **B 65**, 235115. [2] Gillet J.M., Becker P., *J. Phys. Chem. Solids*, 2004, **65**, 2017.

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