Abstract Submitted
for the DAMOP14 Meeting of
The American Physical Society

Interatomic Coulombic decay in nanodroplets
NICOLAS SISOURAT, Universté Pierre et Marie Curie — Interatomic (molecular) Coulombic decay (ICD) is an ultrafast non-radiative electronic decay process for excited atoms or molecules embedded in a chemical environment. Via ICD, the excited system can get rid of the excess energy, which is transferred to one of the neighbors and ionize it. ICD produces two charged particles next to each other and thus leads to Coulomb explosion. Kinetic energy distribution of the ionic fragments gives information on the dynamics of the decay process. From the theoretical point of view general quantum mechanical equations for describing the decay processes and the subsequent fragmentations are known but are only applicable for rather small systems. During the presentation, a semiclassical approach for modeling ICD and the subsequent fragmentations will be presented. This approach involves a classical treatment for the nuclear motion while retaining a quantum description for the electron dynamics. Such approach has low computational costs and can be used to study much larger systems. Comparison of the results from semiclassical and from quantum mechanical calculations will be shown for simple systems, demonstrating the good performance of the semiclassical method. Results on ICD in nanodroplets will finally be reported.

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Date submitted: 03 Feb 2014 Electronic form version 1.4