UNIVERSITÀ DEGLI STUDI DI MILANO

SEMINARI CHIMICI

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Data ***Lunedì 9 Ottobre 2006 ore 16 Aula 206***

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Titolo **Radiation Damage Mechanisms in Biological Systems: Quantum Dynamical Decay after Secondary Electron Capture**

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It is by now well known that high energy radiation can induce damage in liquids and solids via the production of a wide variety of intermediate species that are being formed within nanoscopic volumes along the ionizing tracks. In qualitative terms, one may say that the primary photon interaction (i.e. the absorbed and scattered photons from the impinging radiation) removes electrons from a very broad range of molecular states and of molecular aggregates, stripping them from outer shells and down to the core levels. Such shower of charged particles, however, now looses energy by further causing ionization in the environment through which they are slowed down. They can thus undergo multiple collisions and generate multiple emissions of further electrons which then constitute the secondary electrons emitted at lower energies and, like the primary ones, over a very broad energetic span. At the elementary level, therefore, the formation of a Transient Negative Ion (TNI) by temporary electron attachment to the molecule is followed by energy redistribution and different pathways to dissociative attachment (DA) and dipolar dissociation (DD). They lead in turn to the production of different fragments, both neutral and ionic.
On the strength of our earlier studies on the structure of scattering precursors to dissociative attachment processes mediated by trapped resonant states we have begun to analyse possible TNI formation in biomolecules, beginning with Uracil, Thymine and Guanine.
At the seminar I therefore intend to show that it is indeed possible to carry out essentially ab initio treatments of the quantum scattering dynamics of low-energy electrons trapped by a complicated biomolecule to form specific TNI transient states that provide clear signatures of precursor structures to possible DA decay channels in such systems.

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