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SEMINÁRIO

Data, hora, local *Date, hour, local*	22-06-2010, 12h00 Auditório do ITN / *ITN Auditorium*

Palestrante *Speaker*	Maria del Carmen Michelini	*Dipartimento di Chimica, Università della Calabria, Italy*

Título
Title

Computational studies in actinide chemistry

Theoretical modeling of actinide chemistry is challenging due to the combined effects of relativity and electron correlation, along with the large number of electrons and the many chemically accessible orbitals. Still, theoretical computations, particularly if approached in close cooperation with experimental studies, present a unique opportunity to provide insights into the chemistry of actinide elements. This presentation is divided into two parts. In the first part, an overview of the theory and methods used to study actinide chemistry will be presented, emphasizing the advantages and shortcomings of the most popular approaches. In the second part, some examples of gas-phase reactions of bare and ligated actinide ions with neutral molecules will be discussed. In these gas-phase studies, Density Functional Theory in close interplay with experimental methodologies has been used to provide detailed descriptions of reaction mechanisms.

Brief CV: Maria del Carmen Michelini graduated from the University of La Plata, Argentina in 1996. She obtained her PhD in Chemistry in 2000 from the same University. She then spent four years as a postdoctoral fellow in the Department of Chemistry of the University of Calabria, where she has been a tenured research and teaching associate since 2005. Her main research interests are in computational chemistry and reaction mechanisms; particularly in transition metal, lanthanide and actinide chemistry.