



Instituto de Estructura de la Materia - Ciclo de Seminarios 2012-2013  
**Seminario del Departamento de Física Molecular**

**ON THE MECHANISM OF ATMOSPHERIC IODINE OXIDE  
PARTICLE FORMATION**

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Atmospheric iodine is involved in ozone catalytic destruction and in ultrafine aerosol formation. Coastal macroalgae, phytoplankton and abiotic processes in the ocean surface and sea ice release iodocarbons and inorganic iodine compounds ( $I_2$  and HOI) into the atmosphere, which are then photo-oxidised forming iodine oxides with the ability to polymerise yielding so-called iodine oxide particles (IOPs). A number of experimental and theoretical studies on this phenomenon have been carried out in the past, but the IOP formation mechanism and the role of water and other condensable vapours remain unclear. In this talk, high level *ab initio* calculations of the geometry and thermochemistry of iodine oxides aggregates and water complexes will be presented. These are used in rate theory calculations to estimate rate coefficients and atmospheric lifetimes. This study has been done in collaboration with the John Plane's group at the University of Leeds. Our theoretical results are used to interpret the observations of the new experimental study carried out in Leed, using the TOF-MS technique, where direct evidence of  $I_2O_y$  ( $y=2,3,4,5$ ) in the gas phase is reported for the first time.

**Viernes, 19 de Abril de 2013, 12:00 horas.**

*Sala de Conferencias. Centro de Física "Miguel A. Catalán".*

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