AB INITIO CALCULATIONS ON LOCAL EXCITED STATES OF LANTHANIDE AND ACTINIDE IONS IN SOLIDS

LUIS SEIJO, ZOILA BARANDIARAN, *Universidad Autónoma de Madrid, Departamento de Química, 28049 Madrid, Spain*.

Wavefunction based *ab initio* techniques of molecular quantum chemistry are used in embedded cluster calculations of lanthanide and actinide ions in solids. Explicit considerations of electron correlations, relativistic effects up to spin-orbit coupling, and embedding effects of the solid host are made by means of approximate, though accurate methods, which turn the computations of large manifolds of local excited states affordable. As a result, absorption and emission spectra are modelled with an accuracy good enough so as to provide interpretations of experimental spectra hard to obtain by other means.
The following results are presented: The blue absorption and the yellow luminescence of the phosphor Ce^{3+}-doped YAG, which is used in Solid-State Lighting devices, and the detailed interpretations of the $5f \rightarrow 6d$ absorption spectra of U^{4+}-doped and U^{3+}-doped Cs_2NaYCl_6.