
UNIVERSITÀ DEGLI STUDI DI PADOVA

DIPARTIMENTO DI SCIENZE CHIMICHE

Giovedì 28 gennaio 2010 alle ore 15:30 presso l'Aula G

il Prof. Massimiliano Aschi

del Dipartimento di Chimica Ingegneria Chimica e Materiali

Universita' di L'Aquila

terrà il seminario dal titolo:

**Applications of computational chemistry in the spectroscopy
of complex molecular systems**

La presenza della S.V. sarà molto gradita

Abstract

One of the main goals of theoretical-computational chemistry is the possibility of reproducing, and hence predicting, the spectroscopic signals of complex molecular systems in condensed phase. Beyond the intrinsic computational costs, a straightforward procedure available at this purpose is still absent mainly because of several conceptual difficulties. As a matter of fact, typical spectroscopic signals of a chromophore in liquid solution should be described, at a first approximation as (classical) ensemble averages of transitions occurring within quantum degrees of freedom.

In our laboratory we have developed and applied a new computational methodology aimed at this purpose. In this talk the basic features, the advantages and the limitations of our approach will be presented and discussed in the light of recent results concerning the study of UV and IR absorption spectra of different solutes at the equilibrium.

Il Direttore del Dipartimento

Prof. Antonino Polimeno

Prof. Paolo Scrimin