SEMINAIRE ISMO

Attention ! Jour inhabituel

R. Benny GERBER

Hebrew University of Jerusalem, Israel
and University of California, Irvine, U.S.A.

Unravelling Properties of Large Biological Molecules by First-Principles Spectroscopic Calculations

Vibrational spectroscopy is a sensitive probe of molecular properties, including structure and the intermolecular force field. For large molecules, however, first principles calculations are very challenging beyond the harmonic approximation, due to coupling between different vibrational modes.

In this lecture, we argue that the Vibrational Self-Consistent Field (VSCF) method is a major step forward in the field, making calculations feasible for systems of the size of large peptides.

Applications include:

1. For sugars and hydrated sugar molecules, comparison with experiments leads to determination of the structure and the force field.

2. For long-drain hydrocarbons, agreement with Raman experiments provides understanding of the C-H band spectra, and tools for analyzing CARS imaging of lipids and bio-membranes.

We will show future directions of progress, including applications to structure and interaction of proteins.

* * * * *

Vendredi 21 octobre 2011 à 11 h 00

Bât. 210 – Amphi I (2è étage) (jour inhabituel)

Université Paris-Sud, 91405 ORSAY Cedex