

# Physics Colloquium

Michigan Technological University

Thursday, October 24, 2013

4:00 pm

Room 139 Fisher Hall



**Neutron and Raman spectroscopy studies of the quantum dynamics of hydrogen molecules in simple and binary clathrate-hydrates**

**Dr. Lorenzo Ulivi**

**CNR - Consiglio Nazionale delle Ricerche  
Istituto dei Sistemi Complessi, Sez. Firenze  
Sesto Fiorentino, ITALY.**

**Abstract:** Hydrogen gas and water may form solid clathrate hydrates either with themselves (simple clathrates) or together with a different substance (binary clathrates). Both have raised strong interest recently as possible materials for hydrogen storage. The confinement of the hydrogen molecules is substantially different in the two cases: in binary clathrates hydrogen singly occupies the smaller dodecahedral cages, while in simple clathrates also the larger cages (hexakaidecahedral) are filled with several (up to four) hydrogen molecules. In this talk the results of recent inelastic neutron scattering (INS) and Raman spectroscopy measurements will be presented and discussed. In the high-resolution neutron spectrum of the binary clathrate, the  $H_2$  (or HD) molecule excitations give rise to very strong bands, which are assigned unambiguously to rotational transitions of the  $H_2$  molecule, to center-of-mass translational transitions (rattling in the cage) and to combinations of these. The Raman spectra reveal details of the interaction of the  $H_2$  molecule with the cage, and of the different number of molecules in the cages. An interesting effect, revealed by Raman measurements in hydrogen clathrates at 20 K, is the different rate of conversion from *ortho*- $H_2$  to *para*- $H_2$  for molecules caged alone or in larger number.

**Bio:** Dr. Lorenzo Ulivi is a Senior Scientist at the National Research Council (CNR) in the Institute of Complex Systems Laboratories in Sesto Fiorentino, Italy. He has been a Research Fellow at Max-Planck-Institute for Quantum Optics in Munich, (Germany) and the University of Manitoba, Winnipeg (Canada). He studies molecular solids and materials under extreme pressure using Raman spectroscopy, infrared spectroscopy, x-rays and neutron diffraction. He is co-author of more than 80 papers published in national and international journals, editor of two books, and author of numerous presentations at national and international conferences.