



British Embassy  
Rome

## WORKSHOP

# HIGH-ENERGY NEUTRONS FOR SCIENCE AND SOCIETY

A UK-Italy Workshop  
Rome, 5<sup>th</sup> - 6<sup>th</sup> October 2010  
Villa Wolkonsky, Via Ludovico di Savoia

**16:30**      *Coffee break*

### Session II - NEUTRON EXPERIMENTS

**Chair: Roger Pynn (Indiana University)**

**17:00**      Jerry Mayers (*STFC, ISIS Facility*)  
*What can be learnt from measurements of the momentum distribution of liquid  $^4\text{He}$ ?*

**17:30**      **George Reiter (University of Houston)**  
**title TBD**

**18:00**      Carla Andreani (*University of Rome Tor Vergata*)  
*Proton quantum effects in ice, normal and confined water*

**19:00**      *Cocktail*

### 6<sup>TH</sup> OCTOBER

### Session III- TECHNIQUES AND INSTRUMENTATION WITH HIGH ENERGY NEUTRONS

**Chair: Carla Andreani (University of Rome Tor Vergata)**

**09:00**      **Roberto Senesi (University of Rome Tor Vergata)**  
**title TBD**

**09:30**      Henry Glyde (*University of Delaware*)  
*Bose Einstein Condensation and Superfluidity Investigated Using High-Energy Neutrons*



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- 10:00 Marco Zoppi (*CNR, ISC*)  
*Raman-like scattering using high energy neutrons: applications to hydrogen and hydrogen-containing materials*
- 10:30 *Coffee break***
- 11:00 Robert Mc Greevy (*STFC, ISIS Facility*)  
*Neutrons, science and impact: the potential role of high energy spectroscopy*
- 11:30 Giuseppe Gorini (*University of Milano Bicocca and CNR*)  
*Epithermal neutrons for cultural heritage research*
- 12:00 Chris Frost (*STFC, ISIS Facility*)  
title TBD**
- 12:30 *Lunch***
- 14:00 Round Table and discussion session  
*Present and Future perspectives with High Energy Neutrons*
- 15:00 *Coffee break***
- 15:30 *Close***

## **Raman-like scattering using high energy neutrons: applications to hydrogen and hydrogen-containing materials**

M. Zoppi, M. Celli, D. Colognesi, L. Ulivi

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The extensive use of Raman spectroscopy in the investigation of the internal molecular motions has been one of the most relevant achievements of the last century. Thanks to this experimental technique, thousands of molecular structures have been determined and refined. Nonetheless, the use of photons, mostly in the visible region, has been soon recognized to represent a limiting factor for optically dense materials. The availability of dense beams of high energy neutrons, together with the construction of dedicated spectroscopic instrumentation, has allowed to get rid of this restriction and to take full advantage of the high neutron penetration power in dense matter. Today, the resolving power of neutron instrumentation is not too much dissimilar from that of the corresponding photon instrumentation and the available energy range extends well beyond the eV limit. Thus, allowing to cover the whole vibrational spectrum available to any molecular system.

In this contribution, I will show how a dedicated instrument (TOSCA at ISIS) can be effectively used in neutron spectroscopy applications for the investigation of rotovibrational motions in condensed matter systems. Thus becoming an effective equivalent of a Raman spectrometer, with the invaluable advantage of the neutron penetration power in dense systems.

A further advantage of a dedicated high energy neutron spectrometer is represented by the possibility of exploring the application of the Impulse Approximation limit to the center of mass dynamics of molecular systems. By this technique, taking into account the high incoherent neutron scattering cross section of the proton and the extensive energy range available on TOSCA, a wide research area can be exploited allowing to obtain a direct experimental information on the quantum dynamics of liquid and solid bulk hydrogen. Also, it will be shown how the peculiar characteristics of a dedicated neutron Raman instrument can be exploited in the investigation of the quantum dynamics of molecular hydrogen in the nanoconfined geometry of clathrate hydrates, or in detecting its rotational motion on the surface of a carbon nanotube.

Last, but not least, important applications of this spectroscopic tool to the investigation of hydrogen-storage materials, including simple and complex light metal hydrides, will be outlined.