

MC11: Lattice vibrations: lifetime, transport and (quantum) thermodynamics

Organisateurs : M. Casula, Ph. Depondt, F. Finocchi, L. Paulatto

Vendredi 26 août – 8h30- 12h00

8:30 - 9:00	Unraveling the Ground-State Structure of BaZrO₃ by Neutron Scattering Experiments and First-Principles Calculations
MC11-1	A. Perrichon , E. J. Granhed, G. Romanelli, A. Piovano, A. Lindman, P. Hyltdgaardb, G. Wahnström, M. Karlsson <i>ISIS Neutron and Muon Source, RAL, STFC, Oxfordshire OX11 0QX, United Kingdom. adrien.perrichon@stfc.ac.uk</i>
9:00 - 9:15	Couplage entre phonons et ordre magnétique à courte portée dans le pnicture : BaFe₂Se₃
MC11-2	Marie-Bernadette Lepetit , M. J. Weseloh, V. Balédent, W. Zheng, M. Verseils, P. Roy, J. B. Brubach, D. Colson, A. Forget, P. Foury-Leylekian <i>Institut Néel & Institut Laue Langevin, Grenoble.</i>
9:15 - 9:30	Emergent phenomena in the thermal-radiative response of hBN
MC11-3	Giorgia Fugallo <i>LTeN, UMR 6607, F-44000 Nantes, France. giorgia.fugallo@univ-nantes.fr</i>
9:30 - 9:45	Ab-initio lattice dynamics of strongly anharmonic materials
MC11-4	Ibrahim Buba Garba , Lorenzo Paulatto <i>Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), Sorbonne Université, Paris ; Department of Physics, Federal University Gashua, Yobe State, Nigeria. ibrahim.garba@sorbonne-universite.fr</i>
9:45 - 10:00	aTDEP : Lattice dynamics including anharmonicity
MC11-5	F. Bottin, A. Castellano and J. Bouchet <i>CEA, DAM, DIF, F-91297 Arpajon, France and Université Paris-Saclay, CEA, Laboratoire Matière en Conditions Extrêmes, 91680 Bruyères-le-Châtel, France. francois.bottin@cea.fr</i>

10h00-10h30 Coffee break

**10:30 -
11:00**

Exploring quantum effects in vibrational properties of Lithium at low temperature and high pressure

MC11-6

Sara Bonella

CECAM@EPF-Lausanne, Avenue Forel 2, 1015 Lausanne. sara.bonella@epfl.ch

**11:00 -
11:15**

Wave-particle duality in heat conduction from Wigner's formalism

MC11-7

Michele Simoncelli, Nicola Marzari, and Francesco Mauri

Theory of Condensed Matter Group of the Cavendish Laboratory and Gonville & Caius College, University of Cambridge, United Kingdom. ms2855@cam.ac.uk

**11:15 -
11:30**

Anharmonic phonons in hydrogen-rich materials

MC11-8

Tommaso Morresi, Rodolphe Vuilleumier et Michele Casula

IMPMC, Sorbonne Université, Paris. michele.casula@upmc.fr

**11:30 -
11:45**

Quantum phase diagram of high-pressure hydrogen

MC11-9

Lorenzo Monacelli, Michele Casula, Kosuke Nakano, Sandro Sorella, Francesco Mauri

EPFL, Lausanne, Switzerland. lorenzo.monacelli@epfl.ch

**11:45 –
12:00**

Anharmonic and Nuclear Quantum Effects on vibrational spectra via trajectories

MC11-10

Thomas Plé, Simon Huppert, Philippe Depondt, Sara Bonella and Fabio Finocchi
Sorbonne Université, CNRS, Institut des NanoSciences de Paris, INSP, 4 Place Jussieu, F-75005 Paris, France. depondt@insp.jussieu.fr

Posters

MC11-11 **Phonon anharmonicity at lower mantle conditions: Consequences on the thermal conductivity of MgO**

Saadi Chabane, Paola Giura, Lorenzo Paulatto, Daniele Antonangeli
Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), Sorbonne Université, Paris, France. saadi.chabane@upmc.fr

MC11-12 **Fully quantum investigation of high-Tc sulfur hydride superconductor**

R. Taureau, T. Morresi, and M. Casula
Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), Sorbonne Université, Paris, France. romain.taureau@sorbonne-universite.fr