18èmes Journées de la Matière Condensée
22-26 août 2022, Lyon

Société Française de Physique

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

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

1. **Organisateurs (avec affiliation, usuellement 2 ou 3 personnes) :**
   Michele Casula (IMPMC, Sorbonne Université), Philippe Depondt (INSP, Sorbonne Université), Fabio Finocchi (INSP, Sorbonne Université), Lorenzo Paulatto (IMPMC, Sorbonne Université)

2. **Parrainage ou lien avec des sociétés savantes, des GDR ou autres structures :**

3. **Résumé de la thématique du minicolloque :**
   We propose a miniworkshop on the most recent progress in the study of lattice dynamics. In the last couple of years, we have seen a remarkable development of new theoretical schemes to describe lattice vibrations beyond the harmonic approximation [1,2,3,4]. Phonon-phonon scattering, which originates in a beyond-harmonic framework, is pivotal in determining the materials properties we all experience, such as thermal transport, phase transition mechanisms or thermal expansion. Moreover, anharmonic lattice vibrations are the key to interpret, understand and predict fascinating and less common properties such as ferroelectricity in functional materials. They are also fundamental to understand the thermodynamics of hydrogen-based materials, which have seen a resurgence of interest after the discovery of record-breaking critical temperature superconductivity under high pressure in hydrides. In fact, strong nuclear quantum effects, sustained by the low proton mass, trigger remarkable anharmonic phenomena in these materials and make their phase diagram determination, their vibrational spectrum and their superconducting critical temperature estimate challenging to predict. Recent advances in both theoretical approaches and experimental techniques have paved the way to a more precise quantification of these effects, leading to stricter comparison and feedback between theory and experiment, to enhance the predictive capabilities of *ab initio* based methods and to compare perturbative approaches to semi-classical molecular dynamics. This miniworkshop aims at gathering the main players of the field in the French panorama to foster collaborations and to build up a tighter community.

Références

[1] N.K. Ravichandran and D. Broido, PRB **98**, 085205 (2018).

[2] E. Mangaud, S. Huppert, T. Plé, P. Depondt, S. Bonella,and F. Finocchi, J. Chem. Theory Comput. **15**, 2863 (2019).

[3] L. Monacelli, R. Bianco, M. Cherubini, M. Calandra, I. Errea and F. Mauri, J. Phys.: Condens. Matter **33**, 363001 (2021).

[4] T. Morresi, L. Paulatto, R. Vuilleumier, M. Casula, JCP **154**, 224108 (2021).