Session: Vibrational Properties of Materials

Abstract

Density Functional Theory is essentially a zero Kelvin theory using Born-Oppenheimer approximation [1] to increase its time efficiency, the main reason why it is so popular. Effects of vibrational degrees of freedom of constituent atoms of the system can be introduced through harmonic approximation of the phonons. This approach is good enough to describe some of the phenomena, thermal expansion [2], thermal conductivity [3], temperature band renormalization [4], etc. However for highly anharmonic systems this approximation fails and better and more sophisticated approach is needed, like in the case of structural phase transitions [5,6].

This session will host researchers wanting to present their work on the vibrational properties of materials, such as, but not limited to, thermal conductivity, electron-phonon coupling, thermal expansion, etc.

Invited Speaker

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References

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[3] A. H. Romero *et al*, *Phys. Rev. B* **91**, 214310 (2015)
[4] P. B. Allen and M. Cardona, *Phys. Rev. B* **27**, 4760 (1983)
[5] A. Dewandre *et al*, *Phys. Rev. Lett.* **117** (27), 276601 (2016)
[6] G. A. Ribeiro *et al*, *Phys. Rev. B* **97** (1), 014306 (2018)