UNIVERSITÉ DU LUXEMBOURG

Physics Colloquium

10th of October, 2019 at 9:00 am
Coffee at 8:45 am

Campus Limpertsberg
Bâtiment des Sciences – room BS 0.04

Talk by Prof. Alessio Zaccone
Department of Physics, University of Milan.

Invited by Physics Research Unit.

Lattice dynamics, phonons and mechanics in disordered and dissipative systems

We recently developed a new atomistic calculation methodology which extends lattice dynamics to disordered and "real" solids, called Nonaffine Lattice Dynamics (NALD), based on the concept of nonaffine displacements [1], which are ubiquitous in all real materials (crystals with defects and grain boundaries, glasses etc). This framework also allows one to predict the dynamical mechanical response of "real" materials across the entire time-scale spectrum, thus providing a working solution for the well known problem of bridging time and length scales in the dynamical simulation of materials at the atomic level. The method has been shown to be predictive on the example of a model glassy material of Kremer-Grest polymer chains [2], and recent results extend the description at the atomistic level for real polymer glasses (polyethylene, pDCPD, pNBOH, etc) [3]. Then I will show some recent results [4,5] on the theoretical modelling of phonons and vibrational density of states in solids, both ordered and disordered, where anharmonicity is important. This unifying model, among other things, explains the recent surprising experimental observation (by various experimental groups) of glassy vibrational anomalies in perfectly ordered crystals.

[1] A. Zaccone and E. Scossa-Romano, Phys. Rev. B 83, 184205 (2011).
[2] V.V. Palyulin, C. Ness, R. Milkus, R. Elder, T. W. Sirk, and A. Zaccone, Soft Matter 14, 8475-8482 (2018).
[3] R. M. Elder, A. Zaccone, T. W. Sirk, ACS Macro Letters 8, 1160 (2019).
[4] M. Baggioli and A. Zaccone, Phys. Rev. Lett. 122, 145501 (2019).
[5] M. Baggioli and A. Zaccone, arXiv:1812.07245 .

Biography:

Alessio Zaccone, after undergraduate studies at Politecnico di Torino, obtained a PhD in Chemical Physics at ETH Zurich in 2010. He held academic positions including the Oppenheimer Research Fellowship in the Cavendish Laboratory at University of Cambridge, the Moessbauer Professorship in Physics at Technical University Munich, and a Lectureship in Statistical Physics at University of Cambridge. Currently he is an Associate Professor in the Department of Physics at University of Milan. In 2017 he has been listed by the ACS Industrial & Engineering Chemistry Journal as one of the 37 most influential researchers (with <12 years of independent career) worldwide for impact on chemical sciences. In 2019 he has been elected by the Academy of Science of Goettingen as the Gauss Professor for 2020 at the University of Goettingen.
In 2019 he has been nominated in the Class of 2020 Emerging Leaders in Materials Physics by the IoP Journal of Physics: Materials. Since 2016 Alessio Zaccone is an established collaborator of the government of the USA and leads a research program on atomistic simulations of materials mechanics funded by the US Army Research Laboratory. His research activities lie in the area of theoretical and computational modelling of structurally disordered atomic, molecular and soft materials, with particular emphasis on phononics, mechanics and their link with structure across different length-scales.

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