



Séminaire Invité : Jeudi 10 mars – 10H30

Salle de réunion – Bâtiment 83

Alan McGaughey

Professor of Mechanical Engineering at Carnegie Mellon University



10H00

Phonon properties and thermal conductivity of 3-D and 2-D crystals

Thermal transport in semiconductors is dominated by phonons, quanta of energy associated with atomic vibrations. Advances in computational techniques and power have made it possible to predict the frequencies, group velocities, and lifetimes of individual phonon modes from density functional theory calculations. From these properties, a bottom-up understanding of thermal conductivity can be developed. In this seminar, I will outline the procedure for calculating phonon properties and thermal conductivity and then describe three recent studies from my group : A demonstration of how strain affects phonon properties and thermal conductivity differently in soft and stiff materials, A prediction of strongly-anisotropic thermal conductivity in single-layer black phosphorene, and The separation of the phonon and electron contributions to the thermal conductivity of metals.

Bio :Alan McGaughey is a Professor of Mechanical Engineering at Carnegie Mellon University with a courtesy appointment in Materials Science & Engineering. He holds B. Eng, M. A. Sc., and Ph. D. degrees in mechanical engineering from McMaster University, the University of Toronto, and the University of Michigan. His research group has been supported by the NSF, DOE, AFOSR, and DARPA. He was the Struminger Junior Faculty Fellow in 2009, won a Air Force Office of Scientific Research Young Investigator Program award in 2009, was a Harrington Faculty Fellow at the University of Texas at Austin for 2012-13, and won the Teare Teaching Award at CMU in 2014. He has given invited talks and seminars on modeling atomistic transport across the United States and in Canada, China, France, Japan, Korea, and Singapore.