SEMINAIRE

(de 13 h à 14 h, salle Belledonne, IMEP-LAHC, MINATEC, ouvert aux chercheurs des autres laboratoires)

Jeudi 23 mai 2013

"Predicting thermal conductivity of materials with high precision and at large scale"

by Wu LI

Abstract: The thermal conductivity (κ) is a crucial property of materials in many applications such as thermoelectric, heat management and non-volatile memories. In addition, the knowledge of κ of materials under extreme conditions can help understand the mineral constitution of the earth mantle. On the other hand, parameter-free calculations in materials science are becoming more and more important when searching for new materials with desired functionalities.

In this talk, I will explain how we study materials thermal conductivity by using Boltzmann's transport equation without any adjustable parameters. I will then illustrate this with specific examples of some systems such as Si_xGe_{1-x} and $Mg_2Si_xSn_{1-x}$, which are of particular interest to thermoelectric applications. Special emphasis on the reduction of κ in nanostructures will be made, which is key to the improvement of energy conversion efficiency of the thermoelectric materials. Finally, I will present our results for several hundreds of half-Heusler materials, an example of high-throughput (large scale) study, which is an emerging trend in materials science.

References

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[4] J. Carrete, W. Li, and N. Mingo, S. Wang and S. Curtarolo, *Finding unprecedentedly low thermal conductivity half-Heusler compounds via high-throughput materials modeling*, submitted.

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