



第248回GMSI公開セミナー／第71回CIAiSセミナー

## Ab initio calculations of the lattice thermal conductivity and the discovery of new thermoelectric materials

Professor **Laurent Chaput**

LEMTA, CNRS UMR-7563, Un. Lorraine, Vandoeuvre les Nancy, France

**日時: 2018年3月16日(金) 13:00 - 14:00**  
**場所: 東京大学工学部2号館 72C2号室**

### Abstract :

Within the last few years it has been possible to compute the lattice thermal conductivity of bulk materials using ab initio methods. The interactions between the phonons are obtained from density functional theory and this information is incorporated into the Boltzmann to obtain the thermal conductivity. The good accuracy obtained from those calculations allows trying to use them to find new materials.

We present several strategies that we used performing such a search.

The first method we used is datamining. We screened the entire Material Project library to find materials with ultra low thermal conductivity. The second method is based on polymorphism and was used to study Zn-Sb compounds. Finally we conclude showing how ab initio calculations can be combined with Monte Carlo simulations to describe thermal conduction at the micron scale.



主催:

東京大学大学院工学系研究科「機械システム・イノベーション」プログラム (GMSI)  
「最先端融合科学イノベーション教育研究コンソーシアム」 (CIAiS)

本件連絡先:

東京大学大学院工学系研究科機械工学専攻 教授 塩見 淳一郎

GMSIプログラム事務局 E-mail: [office@gmsi.t.u-tokyo.ac.jp](mailto:office@gmsi.t.u-tokyo.ac.jp) Phone: 03-5841-0696