PCoMS seminar 2022

August 1 (MON.), 2022

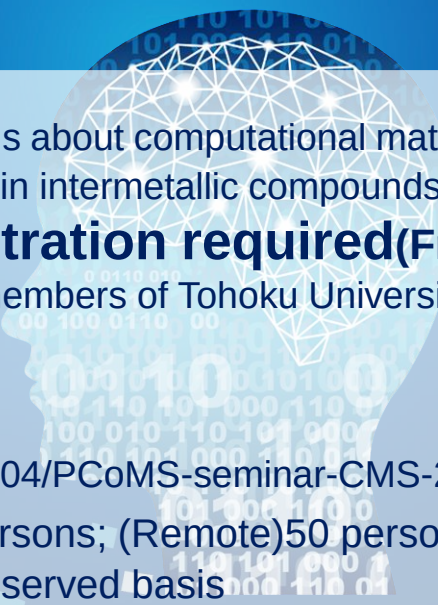
14:00-15:00

Hybrid style meeting

Dr. Jean-Claude Crivello

Univ Paris Est Creteil, CNRS, ICMPE, France

Building thermodynamic database of intermetallic by using massive DFT calculation and supervised machine learning



Main target: Anyone curious about computational materials science, with an interest in intermetallic compounds

Registration Pre registration required(Free of charge):

In-person attendees: Only for members of Tohoku University
by 15:00 on July 20
Remote attendees: Anyone
by 15:00 on July 28
http://pcoms.imr.tohoku.ac.jp/R04/PCoMS-seminar-CMS-22-0801/

Capacity: (In-person)10 persons; (Remote)50 persons; first-come-first-served basis

Place: (In-person) room719, 7th floor, 1st Bldg., Institute for Materials Research, Tohoku Univ. ; (Remote) Zoom

The seminar may be changed to a fully online session depending on the status of the COVID19 infection.

hosted by PCoMS http://pcoms.imr.tohoku.ac.jp/
cooperated by CCMS, IMR, Tohoku Univ. https://www.sc.imr.tohoku.ac.jp/

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Building thermodynamic database of intermetallic by using massive DFT calculation and supervised machine learning

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The heat of formation prediction was the aim of several studies and attempts. In fact, this fundamental value, $\Delta_f H$, is the key parameter in thermodynamics description, such as in the Calphad method. In this latter, the modeling description is well known for addressing the energy of a multicomponent and non-stochiometric phases using the so-called Compound Energy Formalism (CEF) [1]. Applied to an intermetallic phase of s non-equivalent crystallographic sites with a multicomponent n-base, the CEF uses a description where each crystal site is considered as a sublattice and the distribution of every atom generates n^s unique configurations, called end-members, yielding to the need of every $\Delta_f H$ expression.

Based on an independent and unprecedented large first principles dataset, we used a supervised learning approach to predict $\Delta_f H$ of all the possible configurations in two major intermetallic phases: the $L2_1$ Heusler and $D8b$ σ−phase. We conclude from our numerical experiments that the learning database composed of the binary-compositions only, plays the major role in predicting the higher degree system configurations [2]. Our results open a broad avenue to efficient high-throughput investigations of the combinatorial binary computations for multicomponent prediction of complex intermetallic phases, useful to build thermodynamics database.

References

[1] B. Sundman, J. Ågren, *A regular solution model for phases with several components and sublattices, suitable for computer applications*. J. Phys. Chem. Solids (1981), Vol. 42, p. 297-301.

[2] J.-C. Crivello, J.-M. Joubert, *Supervised deep learning prediction of the formation enthalpy of complex phases using a DFT database: The σ−phase as an example*. Computational Materials Science (2022), Vol. 201, p. 110864.

<Notes>

*The members of PCoMS IPD program (fellow and general) can earn 0.5 credit of PCoMS IPD elective course category (A) : Wide knowledge of computational materials science, if he or she attends this seminar and submits the report.