Materials informatics of $D(\varepsilon_{\mathrm{F}})$



Monkeys in 立石寺

ISSP
Mitsuaki Kawamura

Outline

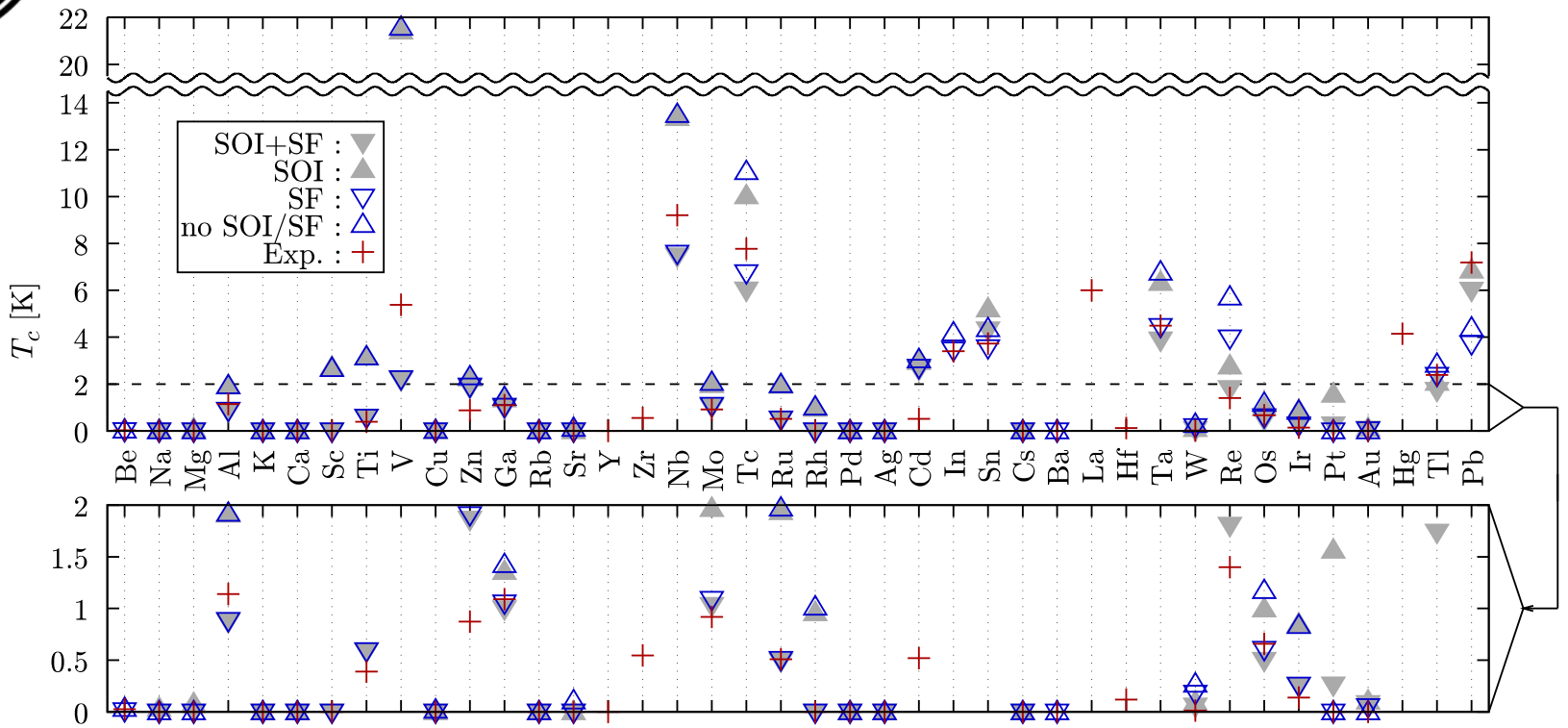
- Motivation
- Method
- Result

Motivation

Find high-T_c superconductor from structure database or newly discovered structures

We can predict T_c fully non-empirically with SCDFT.

Superconducting-Toolkit (SCTK)



Why do we perform machine learning ?

Relatively large numerical cost : $O(N_{\mathrm{atom}}^4)$

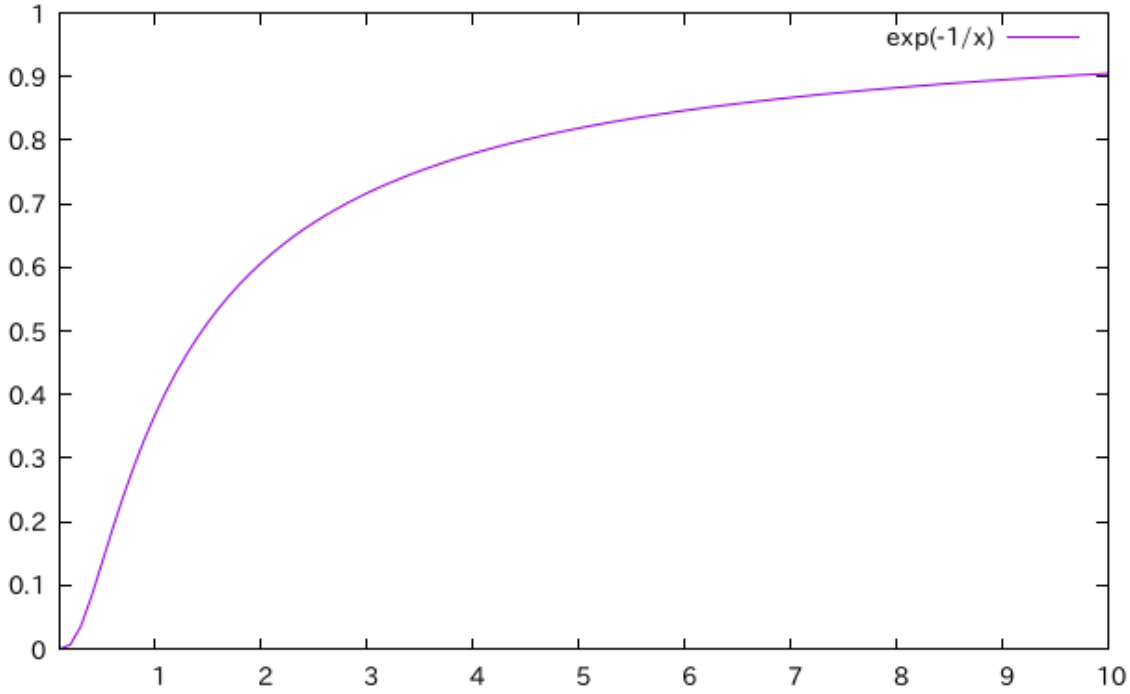
Perform SCDFT only for 100 materials out of 10,000 materials.

Low thermal conductor : A. Seko, *et al.*, PRL 115, 205901 (2015).

In this tutorial, as an exercise,
find large-DOS (per atom) material.

$$T_c \propto \omega_{ph} \exp\left(-\frac{1}{g\,D(\varepsilon_{\mathrm{F}})}\right)$$

BCS theorem



Target

Download CIF file from Crystallographic Open Database

Condition

- Number of atomic species : 1
- Volume of unit cell < 200 Å^3

1,040 materials

Delete duplication and disordered (fractional occupation) system

214 materials

Delete Actinides, Astatine, Radium — 197 materials — Case 1a

Delete Lanthanides — 167 materials — Case 1b

Condition

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Delete duplication, disordered (fractional occupation) system, Actinides, Astatine, Radium, Lanthanides — 227 materials — Case 2

Condition of Bayesian method

- 5 random search for initial guess
- 30 Bayesian steps
- Hyper-parameter tuning at each step

Descriptors

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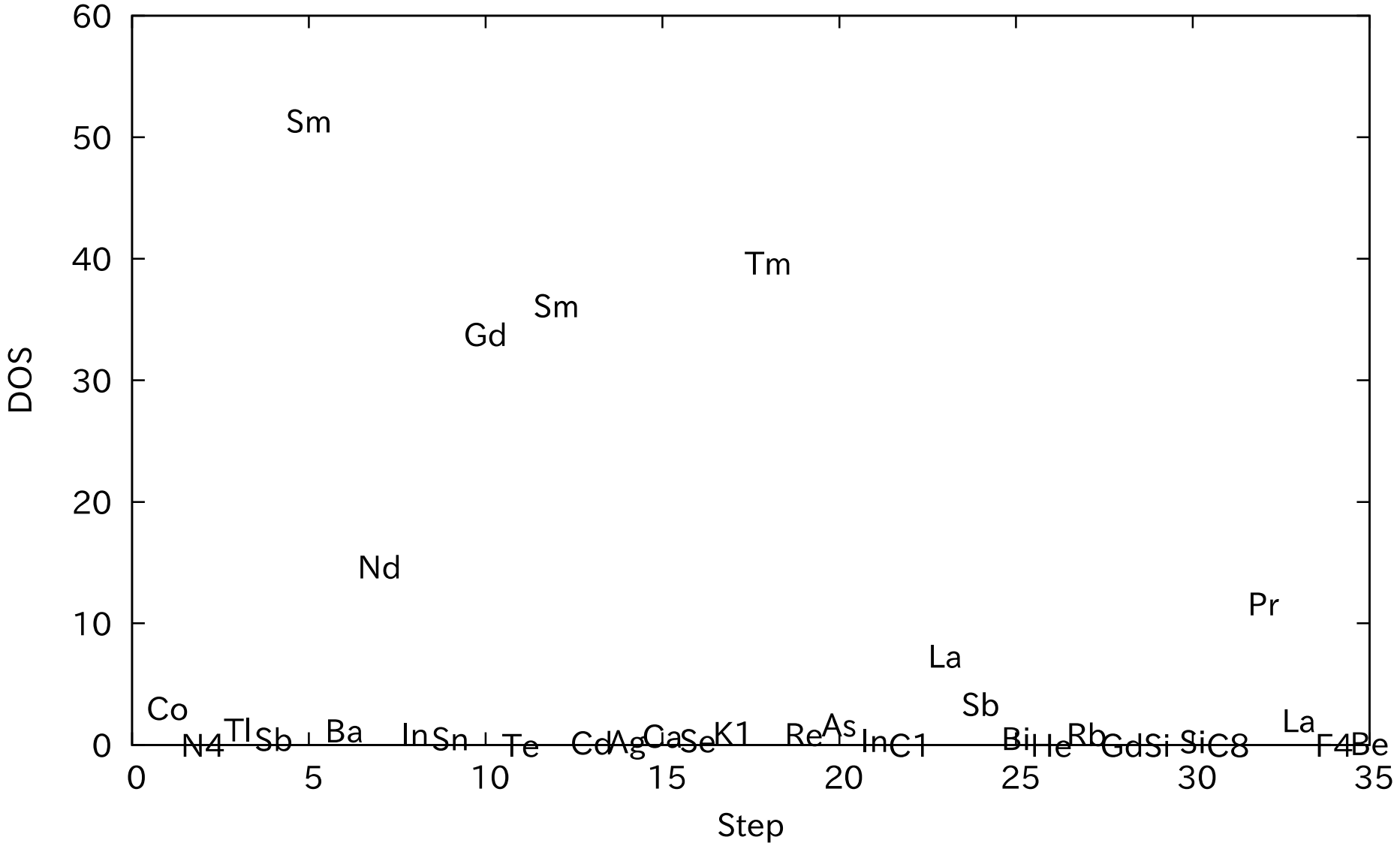
Program packages, numerical conditions

- COMBO, Quantum ESRESSO
- Non-magnetism, w/o structure opt.
- GGA-PBE

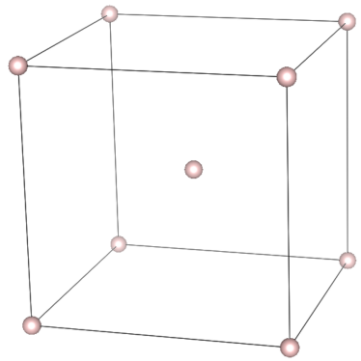
Result : Case 1a

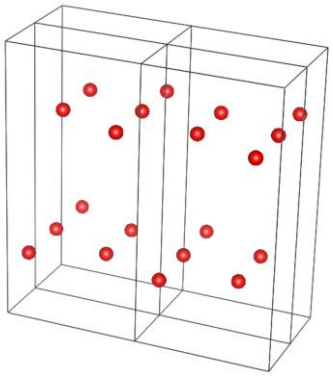
Original : ～15 % Lanthanides

Bayesian : ～26 % Lanthanides



Result : Case 1b





Result : Case 2

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Summary

- Descriptor
- Next : DOS calculation → SCDFT calculation