

DE LA RECHERCHE À L'INDUSTRIE

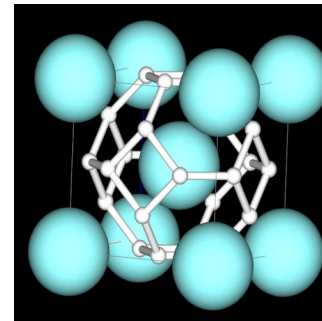


**9TH ABINIT
INTERNATIONAL
WORKSHOP**

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**AB INITIO RANDOM STRUCTURE
SEARCHING METHOD (AIRSS)
AND ABINIT**



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- **New Materials' Prediction: Global challenges**
- **Random Searching Principles**
- **Random Searching implementation**
- **Machine Learning Improvements**

**NEW MATERIALS' PREDICTION
GLOBAL CHALLENGES**

MATERIAL PREDICTION 'S CHALLENGES

Materials Specifications

More efficient , Environmental friendly,
Production Costs

Materials' Prediction Algorithms

Supercomputers



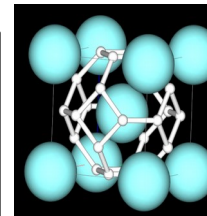
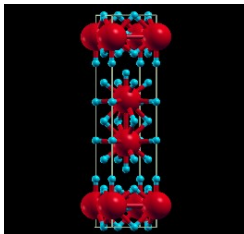
Materials Simulation Software



Big Data and Artificial Intelligence



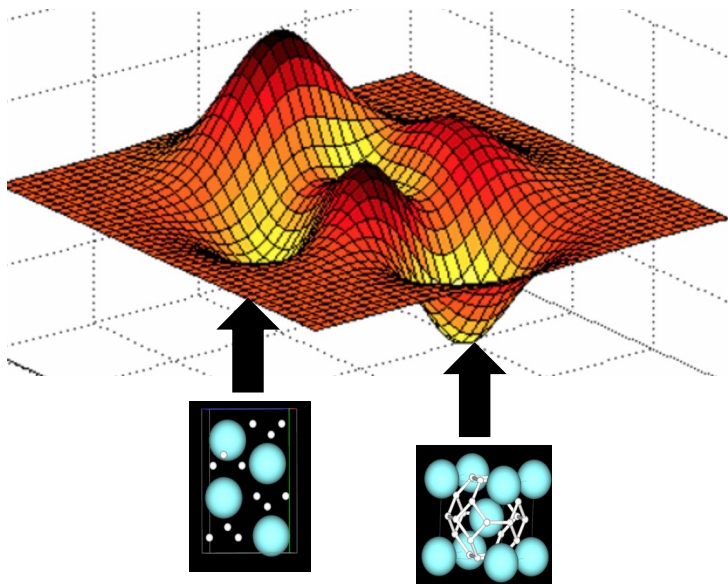
Candidate testing, Experimental Synthesis



GENERAL PRINCIPLES

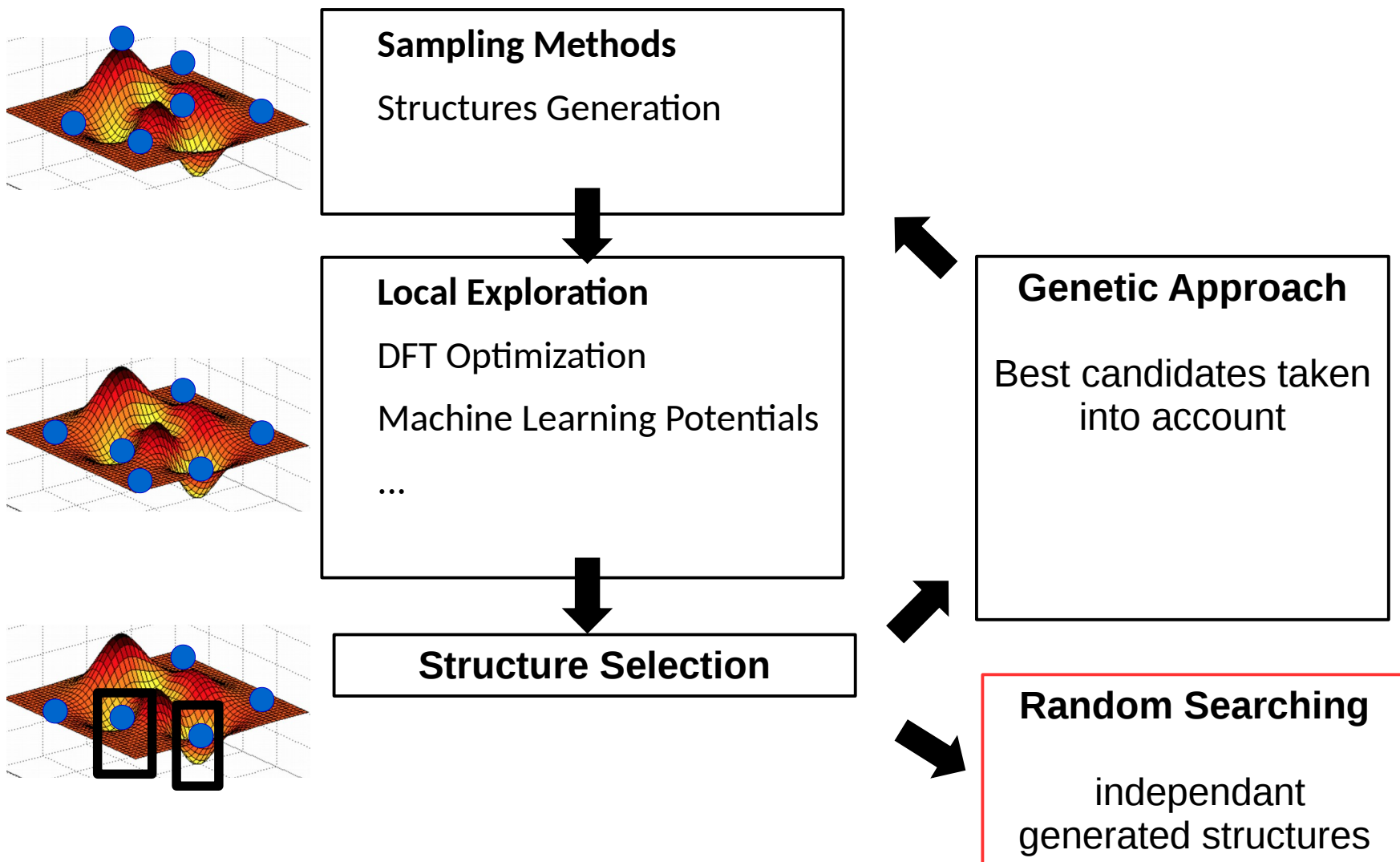
THE POTENTIAL ENERGY SURFACE

- Explore a multidimensional surface to find the global minimum
- Challenging :
 - $3N+6$ dimensions for a given atom number N
 - Exponential increase of the local minima number



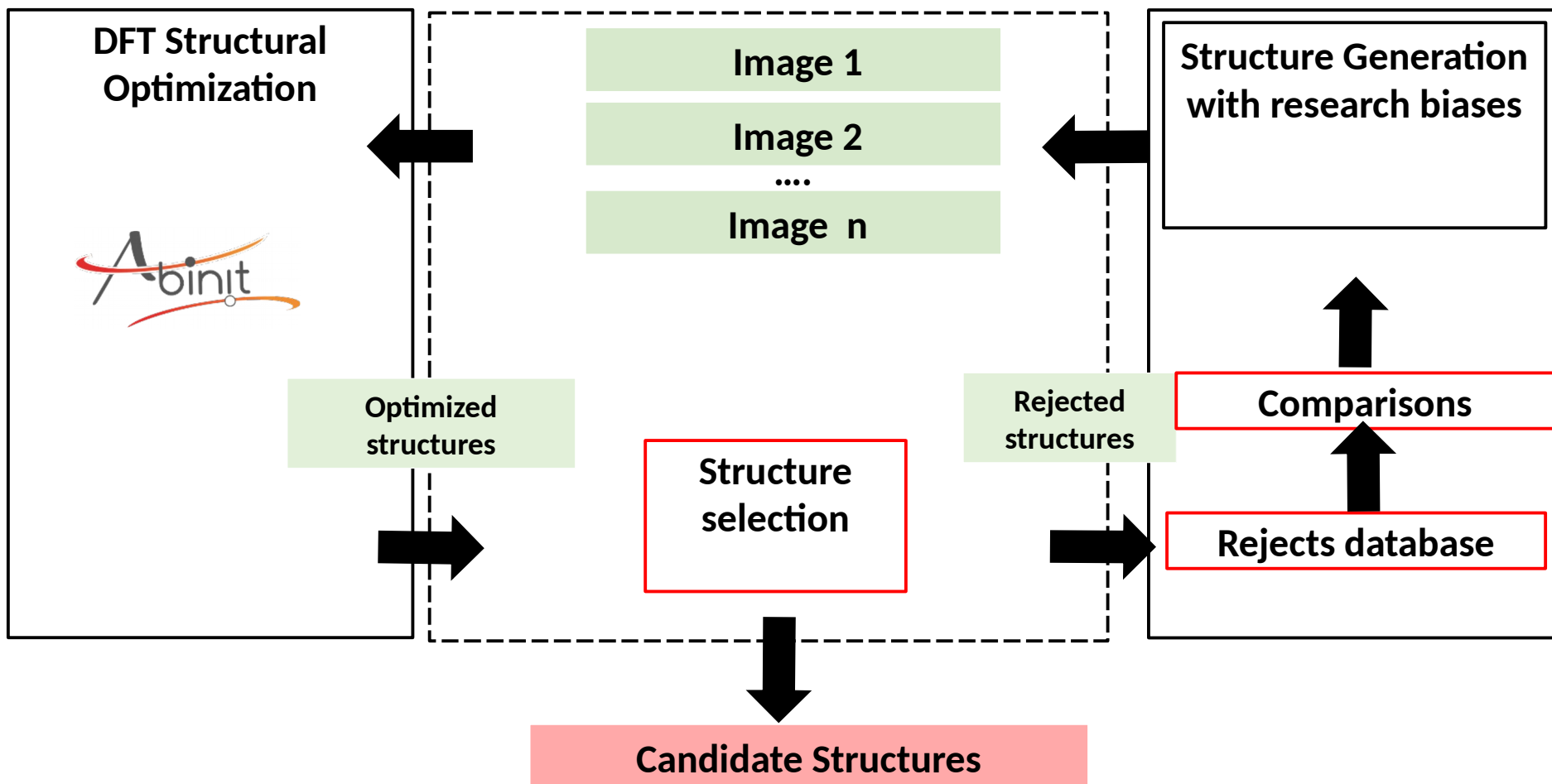
C J Pickard, R J Needs, *Journal of Physics-Condensed Matter*, 23 , 053201 (2011) « Ab initio random structure searching »

POTENTIAL ENERGY SURFACE EXPLORATION

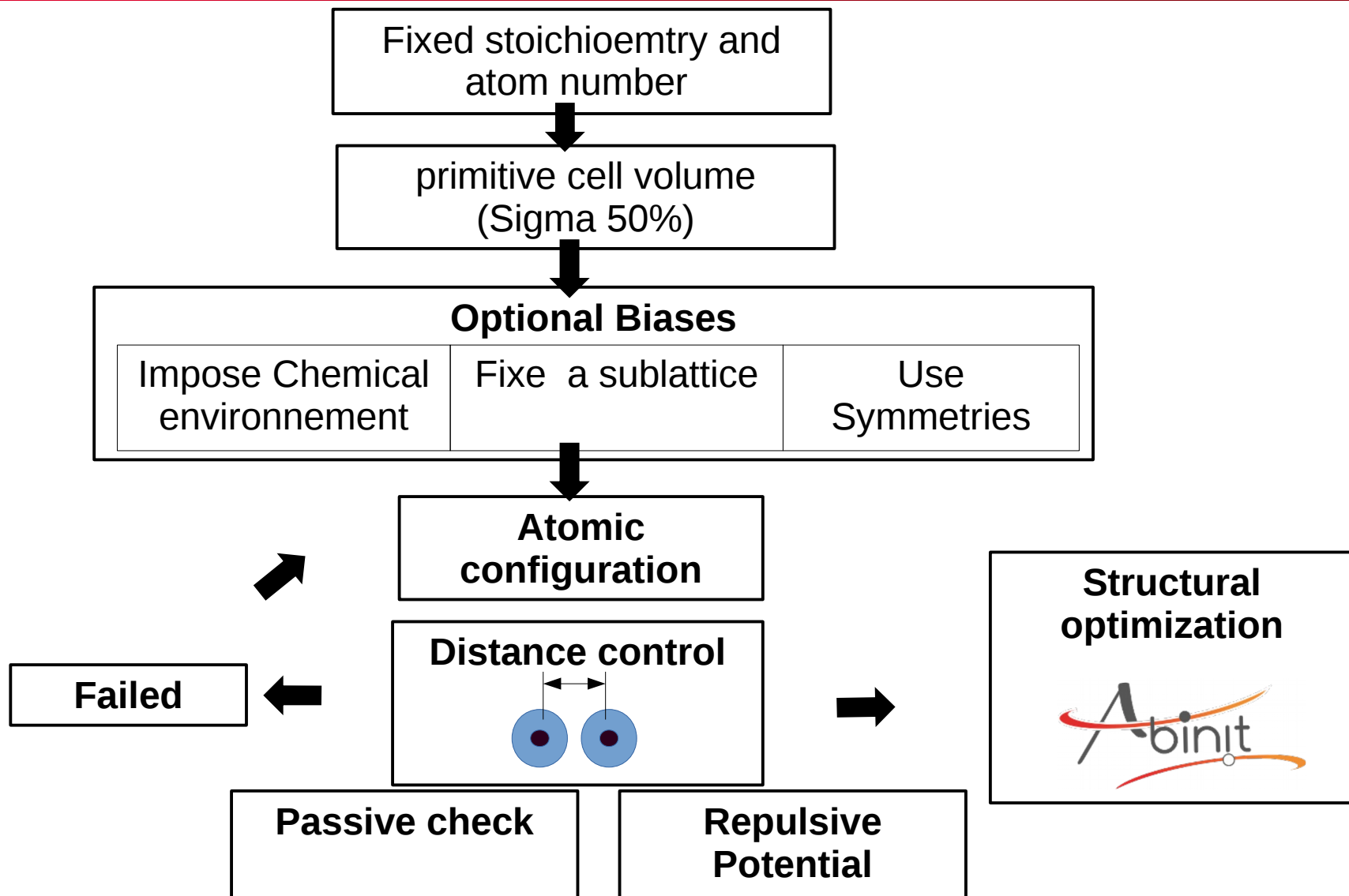


RANDOM SEARCHING IMPLEMENTATION

ABINIT IMPLEMENTATION



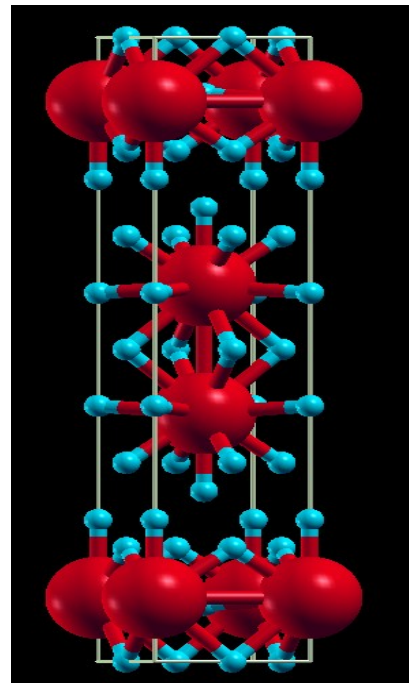
BIASED STRUCTURE GENERATION



APPLICATION TO THE SUPERHYDRIDES

- High density storage of Hydrogen
- Superconductivity

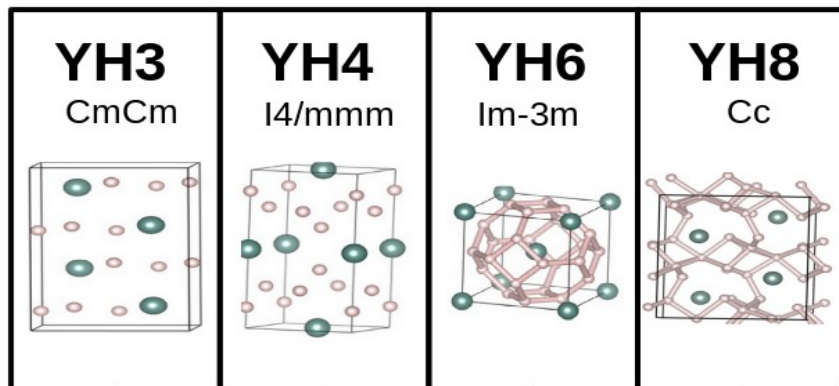
FeH₅ (100 GPa)



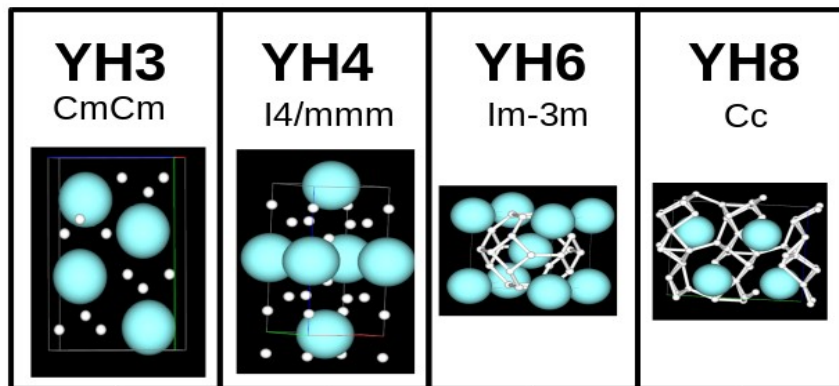
C. M. Pepin, G. Geneste, A. Dewaele, M. Mezouar, P. Loubeyre, *Science* **357**, 382 (2017).

VALIDATION: YTTRIUM HYDRIDES AND SUPERHYDRIDES

Published Reference Structures



Structure Found by AIRSS



100 structures each
More required for repetition

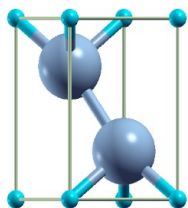
H. Liu, I. Naumov, R. Hoffmann, N. W. Ashcroft, and Russel J. Hemley, PNAS **114**, 6990-6995 (2017)

F. Peng, Y. Sun, C.J. Pickard, R.J. Needs, Q. Wu, and Y. Ma, PRL **119**, 107001 (2017)

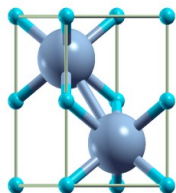
Lu-Lu Liu, Hui-Juan Sun, C Z Wang and Wen-Cai Lu, J.Phys. Condens. Matter **29** (2017)

PREDICTIONS: MANGANESE HYDRIDES AND SUPERHYDRIDES

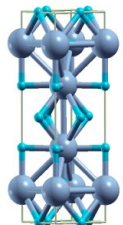
Mn₂H P-3m1



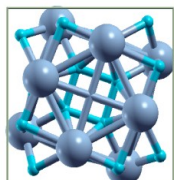
MnH P63/mmc



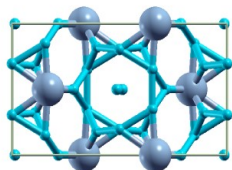
MnH₂ I4/mmm



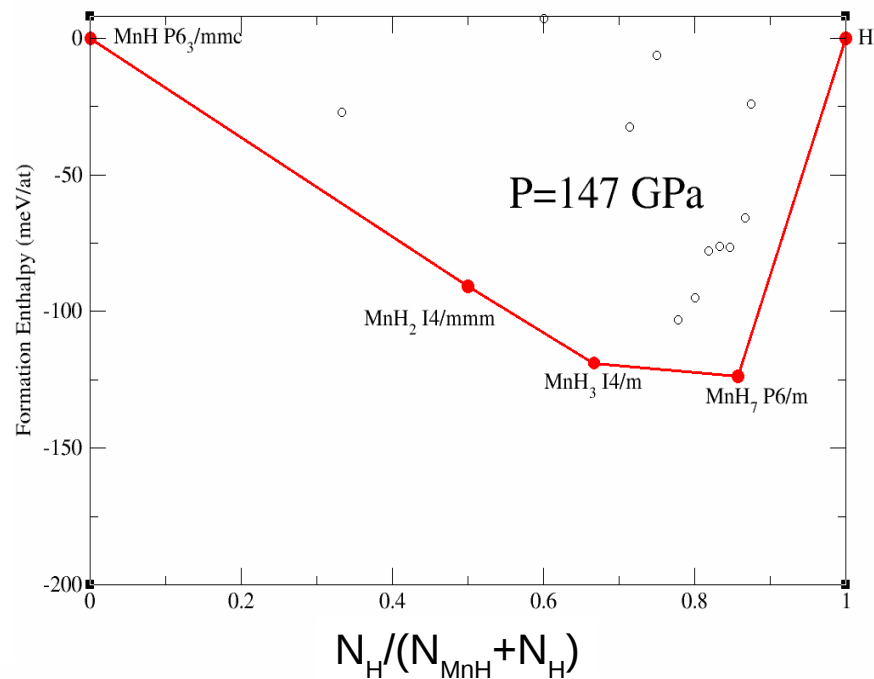
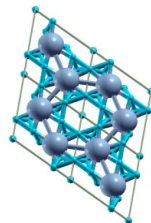
MnH₃ I4/m



MnH₇ C2/m



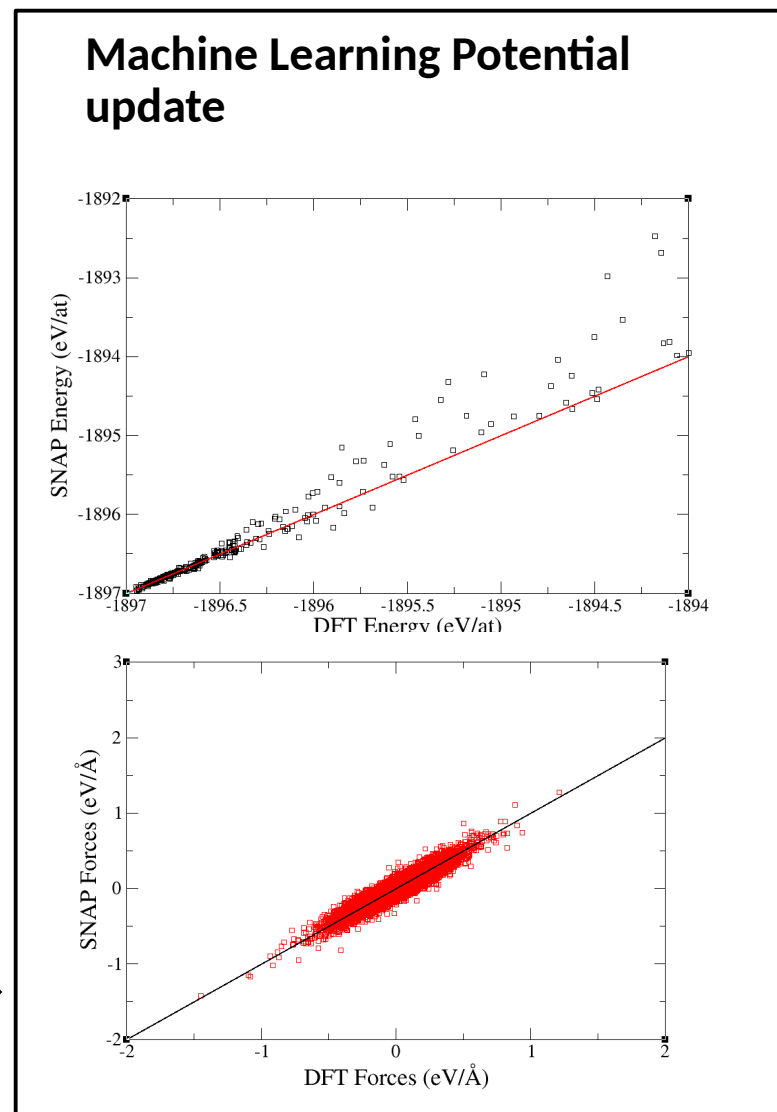
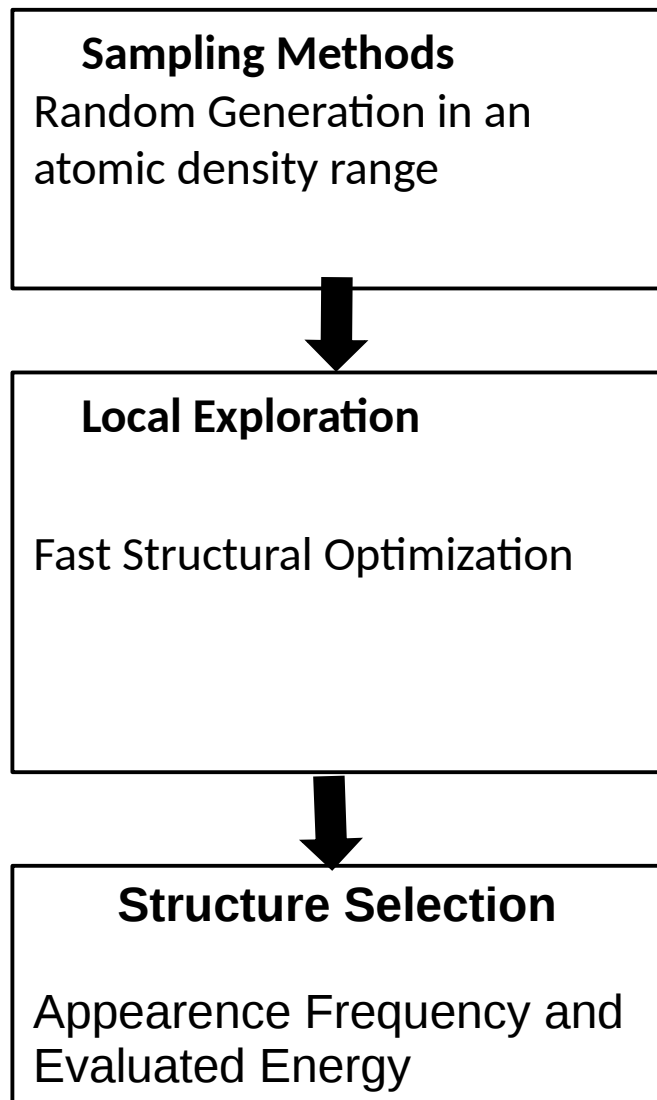
MnH₇ P6/m



New MnH_x structures found with high stability under pressure

**RANDOM SEARCHING IMPROVEMENT
MACHINE LEARNING POTENTIAL**

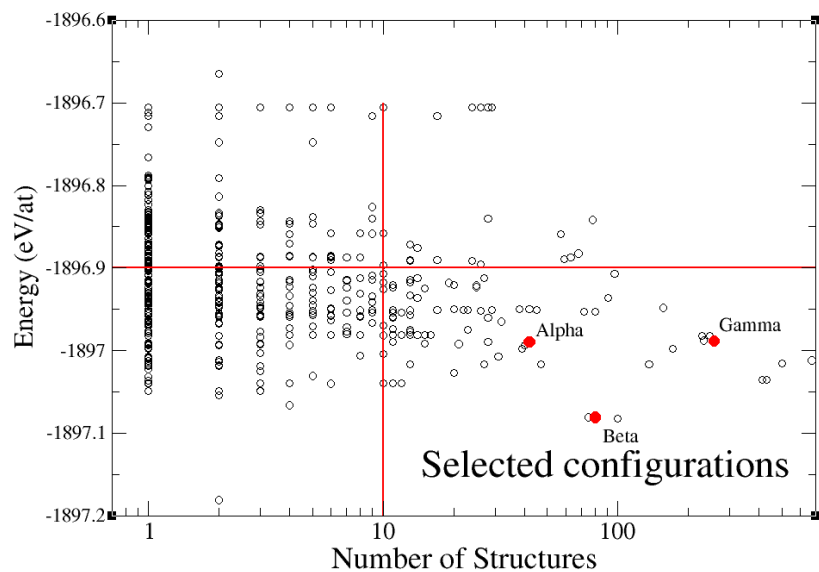
RANDOM SEARCH AND MACHINE LEARNING



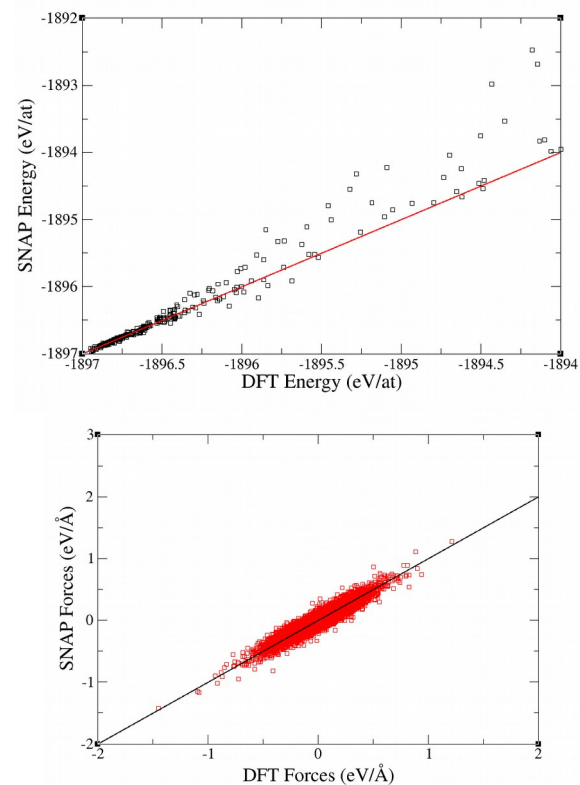
PROOF OF CONCEPT: SN (PRELIMINARY RESULTS)

Spectral Neighbourg Analysis Potential SNAP (Thomson 2017)

The Most Stable Sn Structures have been retrieved in one iteration



Energy-Forces predictions



Two ways to use AIRSS with ABINIT :

- Internal implementation (available in v8.12)
- External scripts

Ongoing improvements:

- Machine Learning
- AbiPy?

Thank you for your attention