AB INITIO RANDOM STRUCTURE SEARCHING METHOD (AIRSS) AND ABINIT

Jean-Baptiste Charraud, Grégory Geneste, Marc Torrent, Jean-Bernard Maillet

CEA, DAM, DIF, F-91297 Arpajon France
OUTLINE

- 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, Environmentally 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

POTENTIAL ENERGY SURFACE EXPLORATION

Sampling Methods
- Structures Generation

Local Exploration
- DFT Optimization
- Machine Learning Potentials
- ...

Genetic Approach
- Best candidates taken into account

Structure Selection

Random Searching
- Independant generated structures
RANDOM SEARCHING
IMPLEMENTATION
ABINIT IMPLEMENTATION

DFT Structural Optimization

Image 1
Image 2
....
Image n

Structure Generation with research biases

Optimized structures

Structure selection

Rejected structures

Comparisons

Rejects database

Candidate Structures
BIASED STRUCTURE GENERATION

Fixed stoichiometry and atom number

primitive cell volume (Sigma 50%)

Optional Biases

- Impose Chemical environment
- Fix a sublattice
- Use Symmetries

Atomic configuration

Distance control

Failed

Passive check

Structural optimization

Repulsive Potential

9th ABINIT International Workshop | 22 Mai 2019 | PAGE 10
APPLICATION TO THE SUPERHYDRIDES

- High density storage of Hydrogen
- Superconductivity

FeH\textsubscript{5} (100 GPa)

VALIDATION: YTTRIUM HYDRIDES AND SUPERHYDRIDES

Published Reference Structures

<table>
<thead>
<tr>
<th>YH3</th>
<th>YH4</th>
<th>YH6</th>
<th>YH8</th>
</tr>
</thead>
<tbody>
<tr>
<td>CmCm</td>
<td>I4/mmm</td>
<td>Im-3m</td>
<td>Cc</td>
</tr>
</tbody>
</table>

Structure Found by AIRSS

<table>
<thead>
<tr>
<th>YH3</th>
<th>YH4</th>
<th>YH6</th>
<th>YH8</th>
</tr>
</thead>
<tbody>
<tr>
<td>CmCm</td>
<td>I4/mmm</td>
<td>Im-3m</td>
<td>Cc</td>
</tr>
</tbody>
</table>


100 structures each
More required for repetition
New MnHx structures found with high stability under pressure.
RANDOM SEARCHING IMPROVEMENT
MACHINE LEARNING POTENTIAL
RANDOM SEARCH AND MACHINE LEARNING

**Sampling Methods**
Random Generation in an atomic density range

**Local Exploration**
Fast Structural Optimization

**Structure Selection**
Appearance Frequency and Evaluated Energy

**Machine Learning Potential update**
The Most Stable Sn Structures have been retrieved in one iteration

Energy-Forces predictions

- SNAP Energy (eV/atoms)
- DFT Energy (eV/atoms)
- SNAP Forces (eV/Å)
- DFT Forces (eV/Å)
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