The Multibinit project

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CESAM / Q-MAT

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Understanding and engineering functional properties often require understanding materials at the atomic scale.

- From \textit{ab-initio} data to second-principles.
- Integrate some degrees of freedom.
- Access relevant properties at operating conditions from different length-scales.
2. Multibinit

Atoms

\[ E = \sum_{ij} C_{ij} u_i u_j \]

DDB XML

Harm + Strain

MODGEN

MD XML

Anharm

Harm + Strain Projection MODES

Anharm Projection ABINIT

Fit MAGNETIC MODEL

Harm DFPT XML WANNIER FUNCTIONS TB+LATTICE COUPLING

Scale-Up ELECTRONIC

Common abstract F03 objects

PIMD MD-spin External modules MC MD Analysis - (q)Agate JB+MS+AM WL-d-H XH JJ+PG+MS

J. Bieder

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2. Multibinit

\[ E = \sum_{ij} C_{ij} u_i u_j \]

\[ E = \sum_{ij} A_{ij} \xi_i \xi_j \]

- **Atoms**
  - Harm + Strain
  - MODGEN
  - DDB
  - XML
  - MD
  - XML

- **Modes**
  - Harm + Strain
  - MODES
  - ABINIT
  - Fit
  - Anharm
  - Projection

**External modules**
- MD-spin
- Analysis - (q)Agate
- JB+MS+AM
- WL-d-H
- JJ+PG+MS

**Software**
- MODGEN
- ABINIT
- Anharm
- Projection
- DDB
- XML
2. Multibinit

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\[ E = \sum_{ij} C_{ij} u_i u_j \]

Modes

\[ E = \sum_{ij} A_{ij} \xi_i \xi_j \]

Spins

\[ E = \sum_{ij} J_{ij} S_i S_j \]

DDB

XML

MODGEN

Anharmonic

Harm + Strain

Projection

MAGNETIC
MODEL

DFPT

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Harm

Fit
2. Multibinit

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  - **MD**
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  - **Projection**

- **ABINIT**
  - **Fit**
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**Spins**

\[ E = \sum_{ij} J_{ij} S_i S_j \]

- **MAGNETIC MODEL**
  - **DFPT**
  - **XML**

**Electrons**

- **WANNIER FUNCTIONS**
  - **TB+LATTICE COUPLING**
  - **Scale-Up**
  - **ELECTRONIC MODULE**

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**Common abstract F03 objects**

- **PIMD**
- **MD-spin**
- **External modules**
- **MC-MD-Analysis**
- **(q)Agate**
- **JB+MS+AM**
- **WL-d-H**
- **XH**
- **JJ+PG+MS**

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*J. Bieder*
2. Multibinit

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Electrons

\[ \text{Harm} + \text{Strain} \]

\[ \text{Harm} + \text{Strain} \]

\[ \text{Harm} \]

\[ \text{Common abstract F03 objects} \]
2. Multibinit

Atoms

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Harm + Strain

DDB
XML
MODGEN
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Modes

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Harm + Strain

MODES
Projection

Abinit
Anharmonic

Spins

$E = \sum_{ij} J_{ij} S_i S_j$

Magnetic Model

DFPT
XML
Projection

Electrons

WANNIER FUNCTIONS
TB+LATTICE COUPLING
Scale-Up
ELECTRONIC MODULE

Common abstract F03 objects

MD
MC
PIMD
MD-spin
External modules

Analysis - (q)Agate

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2. Multibinit

Atoms

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Harm + Strain

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Fit

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Modes

\[ E = \sum_{ij} A_{ij} \xi_i \xi_j \]

Harm + Strain

Projection

Magnetic Model

Modes

Spins

\[ E = \sum_{ij} J_{ij} S_i S_j \]

Harm

Scaling

Electrons

WANNIER

FUNCTIONS

TB+LATTICE

COUPLING

Scale-Up

ELECTRONIC

MODULE

Common abstract F03 objects

External modules

Analysis - (q)Agate

MD

MC

PIMD

MD-spin

{245, 289, 500, 562}
2. Multibinit

**Atoms**

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- Anharmonic

**Modes**

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- Harm + Strain
- MODES
- Projection
- ABINIT
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**Spins**

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- MAGNETIC MODEL
- DFPT
- XML
- Harm

**Electrons**

- WANNIER FUNCTIONS
- TB+LATTICE COUPLING
- Scale-Up
- ELECTRONIC MODULE

**Common abstract F03 objects**

- MD
- MC
- PIMD
- MD-spin
- Analysis - (q)Agate

**External modules**
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MODES

MODES Projection

ABINIT

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MAGNETIC MODEL

Harm

DFPT XML

**Electrons**

\[ \text{WANNIERS} \]

\[ \text{FUNCTIONS} \]

\[ \text{TB+LATTICE COUPLING} \]

\[ \text{Scale-Up ELECTRONIC MODULE} \]

Common abstract F03 objects

MD MC PIMD MD-spin

Analysis - (q)Agate

External modules

Analysis - (q)Agate

External modules

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2. Multibinit

**Atoms**

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**Electrons**

Common abstract F03 objects

- **Harm + Strain**
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- **J. Bieder**

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2. Multibinit

Multibinit in the package

- Multibinit is a new executable included in the `src/98_main/multibinit`
- New directory `src/78_effpot` have been created with many new files!
  - New directory structure is planned to better organize the code
  - Split abstract layer from each potential
  - Split the mover from the potentials
- New input have been created (mix between anaddb and ABINIT)
- The parsing of the XML file is done with Fortran or LibXML (more efficient...)
- MPI Parallelization
- Hybrid Monte Carlo is implemented
- Some of abinit movers are used
- New automatic tests in the version 8
- New documentation with a topic on the website.
- New tutorial to learn how to use multibinit (lattice and spin)
3. Lattice Effective Hamiltonians

Basic Procedure

- Express energy as low order Taylor expansion
  - Use high-symmetry reference structure
  - Variables: local modes and strains
- Determine coefficients from a limited number of DFT calculations
- Resulting energy expansion allows for finite temperature Monte Carlo

Successful results already for many oxide systems.
However identifying a small set of degrees of freedom is often difficult.

We need a general description of the energetics of all the atomic degrees of freedom

W. Zhong et al., PRL 73, 1861 (1994); PRB 52, 6301 (1995)
3. Lattice Effective Hamiltonians

Energy changes around reference structure due to distortions

\[ E_{\text{eff}}(\{u_i\}, \eta) = E_p(\{u_i\}) + E_s(\eta) + E_{sp}(\{u_i\}, \eta) \]

3. Lattice Effective Hamiltonians

Energy changes around reference structure due to distortions

\[ E_{\text{eff}}(\{u_i\}, \eta) = E_p(\{u_i\}) + E_s(\eta) + E_{\text{sp}}(\{u_i\}, \eta) \]

Energy change due to strain only

\[ E_s^{\text{Harm}}(\eta) \]

3. Lattice Effective Hamiltonians

Energy changes around reference structure due to distortions

\[ E_{\text{eff}}(\{u_i\}, \eta) = E_p(\{u_i\}) + E_s(\eta) + E_{sp}(\{u_i\}, \eta) \]

Energy change from atomic displacements

\[ E_p^{\text{Harm}}(\{u_i\}) + E_p^{\text{Anharm}}(\{u_i\}) \]

Energy change due to strain only

\[ E_s^{\text{Harm}}(\eta) \]

3. Lattice Effective Hamiltonians

Energy changes around reference structure due to distortions

\[ E_{\text{eff}}(\{u_i\}, \eta) = E_p(\{u_i\}) + E_s(\eta) + E_{sp}(\{u_i\}, \eta) \]

Energy change from atomic displacements

\[ E_{p,\text{Harm}}(\{u_i\}) + E_{p,\text{Anharm}}(\{u_i\}) \]

Energy change due to strain only

\[ E_{s,\text{Harm}}(\eta) \]

\[ E_{p,SR}(\{u_i\}) + E_{p,LR}(\{u_i\}) \]

3. Lattice Effective Hamiltonians

Energy changes around reference structure due to distortions

\[ E_{\text{eff}}(\{u_i\}, \eta) = E_p(\{u_i\}) + E_s(\eta) + E_{sp}(\{u_i\}, \eta) \]

- Energy change from atomic displacements
  \[ E_p^{\text{Harm}}(\{u_i\}) + E_p^{\text{Anharm}}(\{u_i\}) \]

- Energy change due to strain only
  \[ E_s^{\text{Harm}}(\eta) \]

- Strain-phonon coupling
  \[ E_{sp}^{\text{Harm}}(\{u_i\}, \eta) + E_{sp}^{\text{Anharm}}(\{u_i, \eta\}) \]

3. Lattice Effective Hamiltonians

Energy changes around reference structure due to distortions

\[ E_{\text{eff}}(\{u_i\}, \eta) = E_p(\{u_i\}) + E_s(\eta) + E_{sp}(\{u_i\}, \eta) \]

Energy change from atomic displacements

\[ E_p^{\text{Harm}}(\{u_i\}) + E_p^{\text{Anharm}}(\{u_i\}) \]

Energy change due to strain only

\[ E_s^{\text{Harm}}(\eta) \]

Strain-phonon coupling

\[ E_{sp}^{\text{Harm}}(\{u_i\}, \eta) + E_{sp}^{\text{Anharm}}(\{u_i, \eta\}) \]

Same framework as \( H_{\text{eff}} \) but includes all-atomic degrees of freedom.

3. Lattice Effective Hamiltonians

Phonon term $E_p (\{u_i\}) = E_p^{\text{Harm}} (\{u_i\}) + E_p^{\text{Anharm}} (\{u_i\})$

Taylor development around the reference structure

$$E_p (\{u_i\}) = \frac{1}{2} \sum_{i \alpha j \beta} K_{i \alpha j \beta}^{(2)} u_{i \alpha} u_{j \beta} + \frac{1}{6} \sum_{i \alpha j \beta \gamma} K_{i \alpha j \beta \gamma}^{(3)} u_{i \alpha} u_{j \beta} u_{k \gamma} + O(u^4)$$

with $K_{i \alpha j \beta \gamma}^{n} = \frac{\partial^n E_{\text{eff}}}{\partial u_{i \alpha} \partial u_{j \beta} \cdots} \bigg|_{\eta=0}$.

- Must comply the Acoustic Sum Rule → difficulte to enforce for $n > 2$
- Use displacement differences → ASR satisfied by construction

$$E_{\text{Harm}} (\{u_i\}) = \frac{1}{2} \sum_{i,j,k,h \atop \alpha, \beta} \tilde{K}_{i \alpha j \beta \gamma}^{(2)} (u_{i \alpha} - u_{j \alpha})(u_{k \beta} - u_{h \beta})$$

3. Lattice Effective Hamiltonians

\[ E_p^{\text{Harm}} (\{ u_i \}) = E_{p,SR}^{\text{Harm}} (\{ u_i \}) + E_{p,LR}^{\text{Harm}} (\{ u_i \}) \]

\[ E_p^{\text{Harm}} (\{ u_i \}) = \frac{1}{2} \sum_{i \alpha j \beta} K_{i \alpha j \beta} u_{i \alpha} u_{j \beta} = \frac{1}{2} \sum_{i \alpha j \beta} (S_{i \alpha j \beta} + L_{i \alpha j \beta}) u_{i \alpha} u_{j \beta} \]

\[ = \frac{1}{2} \sum_{i \in \text{SC}} u_{i \alpha} \sum_{j \in \text{SR}} S_{i \alpha j \beta} u_{j \beta} + \frac{1}{2} \sum_{i \in \text{SC}} u_{i \alpha} \sum_{j \in \text{SC}} \left( \sum_{b} L_{i \alpha j \beta}(b) \right) \frac{u_{j \beta}^b}{u_{j \beta}^{\ell_{i \alpha j \beta}(q=0)}} \]
3. Lattice Effective Hamiltonians

\[ E^{\text{Harm}}_p (\{u_i\}) = E^{\text{Harm}}_{p,SR}(\{u_i\}) + E^{\text{Harm}}_{p,LR}(\{u_i\}) \]

\[ E^{\text{Harm}}_p (\{u_i\}) = \frac{1}{2} \sum_{i \alpha j \beta} K^{(2)}_{i \alpha j \beta} u_{i \alpha} u_{j \beta} = \frac{1}{2} \sum_{i \alpha j \beta} (S_{i \alpha j \beta} + L_{i \alpha j \beta}) u_{i \alpha} u_{j \beta} \]

\[ = \frac{1}{2} \sum_{i \in \text{SC}} u_{i \alpha} \sum_{j \in \text{SR}} S_{i \alpha j \beta} u_{j \beta} + \frac{1}{2} \sum_{i \in \text{SC}} u_{i \alpha} \sum_{j \in \text{SC}} \left( \sum_{b} L_{i \alpha j \beta}(b) \right) \begin{array}{c} b \sum_{b} \end{array} \begin{array}{c} u_{j \beta} \end{array} \]

\[ \tilde{L}_{i \alpha j \beta}(q=0) \]

\[
\begin{array}{cccc}
\text{SR} < \text{LR} & \text{LR} & 0 & 0 \\
0 & \text{SR} & 0 & 0 \\
0 & 0 & 0 & 0 \\
\end{array}
\]

\[
\begin{array}{cccc}
\text{LR} < \text{SR} & \text{LR} & 0 & 0 \\
0 & \text{SR} & 0 & 0 \\
0 & 0 & 0 & 0 \\
\end{array}
\]
3. Lattice Effective Hamiltonians

\[ E_p^{\text{Anharm}} (\{u_i\}) \]

- Anharmonicity degree: chose from maximum order: 3, 4, 5, 6, ...
- For each order build the possible terms

\[
E_p^{(n)} (\{u_i\}) = \frac{1}{n!} \sum_{i,j,k,l,m,n,\ldots,\alpha,\beta,\gamma,\ldots} K_{ijklmn}^{(n)\alpha\beta\gamma} (u_{i\alpha} - u_{j\alpha}) (u_{k\beta} - u_{l\beta}) (u_{m\gamma} - u_{n\gamma}) \ldots
\]

- ASR enforces by using differences
- Too many terms for “high” orders
- Use symmetries to reduce the number of coefficients
3. Lattice Effective Hamiltonians

\[ E_p^{\text{Anharm}} \left( \{ \mathbf{u}_i \} \right) \]

Symmetry considerations: “Symmetry adapted terms”

The operations of the space group can generate a collection of symmetry related terms which reduces the number of independent parameters. In practice:

- Define range or cutoff radius
- Build all terms within this range
- Apply all symmetries to find relations between terms:

\[
(u_{0Bx} - u_{0O3x})^2 (u_{0By} - u_{0O3y})^2 + \frac{\pi}{2} \text{ rotation about the y-axis transforms to } (u_{0Bz} - u_{0O1z})^2 (u_{0By} - u_{0O1y})^2 \\
\rightarrow 15 \text{ independent parameters}
\]

(1\textsuperscript{st} nearest neighbors at 3\textsuperscript{rd} and 4\textsuperscript{th} order in \( u \)) for the anharmonic phonon part.
3. Lattice Effective Hamiltonians

Phonon term $E_p(\{u_i\}) = E_p^{Harm}(\{u_i\}) + E_p^{Anharm}(\{u_i\})$

Harmonic terms

- $K^{(2)}$ obtained by DFPT as the back-Fourier-transformed dynamical matrix
- Remove dipole-dipole interaction in real space to obtain the SR only.
- Use ewald summation to compute the exact dipole-dipole interaction.

⇒ Harmonic terms exact by construction and include all phonon branches
3. Lattice Effective Hamiltonians

Phonon term $E_p(\{u_i\}) = E_p^{Harm}(\{u_i\}) + E_p^{Anharm}(\{u_i\})$

**Harmonic terms**
- $K^{(2)}$ obtained by DFPT as the back-Fourier-transformed dynamical matrix
- Remove dipole-dipole interaction in real space to obtain the SR only.
- Use ewald summation to compute the exact dipole-dipole interaction.
  ⇒ Harmonic terms exact by construction and include all phonon branches

**Anharmonic terms**
- Displacement differences expression allows for an unconstrained optimization of $\tilde{K}^{(n)}$
- Determined by fitting key quantities to limited number of DFT calculations (training set)
3. Lattice Effective Hamiltonians

Strain term $E_s(\eta)$
Taylor development around the reference structure

$$E_s(\eta) = \frac{N}{2} \sum_{ab} C_{ab}^{(2)} \eta_a \eta_b + \frac{N}{6} \sum_{abc} C_{abc}^{(3)} \eta_a \eta_b \eta_c + O(\eta^4)$$

with $C_{ab\ldots}^{(m)} = \frac{1}{N} \left. \frac{\partial^m E_{\text{eff}}}{\partial \eta_a \partial \eta_b \ldots} \right|_{u_i=0}$

- Harmonic term calculated directly: the frozen ion elastic constants (DFPT)
- Anharmonic terms: in practice not required for semi-quantitative results

3. Lattice Effective Hamiltonians

Strain-Phonon coupling \( E_{sp}(\{u_i\}, \eta) \)

Taylor development also subject to ASR

\[
E_{sp}(\{u_i\}, \eta) = \frac{1}{2} \sum_a \sum_{i\alpha} \Lambda^{(1,1)}_{ai\alpha} \eta_a u_{i\alpha} + \frac{1}{6} \sum_a \sum_{i\alpha j\beta} \Lambda^{(1,2)}_{ai\alpha j\beta} \eta_a u_{i\alpha} u_{j\beta} + \ldots
\]

- Forces at homogeneous strain
- Change in force constants with strain

- The \( \Lambda^{(m,n)} \) must comply with a set of ASRs
- Use displacement differences

\[
E_{sp}(\{u_i\}, \eta) = \frac{1}{2} \sum_a \sum_{ij\alpha} \Lambda^{(1,1)}_{ai\alpha} \eta_a (u_{i\alpha} - u_{j\alpha})
\]

\[
+ \frac{1}{6} \sum_a \sum_{ij\alpha kh\beta} \Lambda^{(1,2)}_{ai\alpha j\beta} \eta_a (u_{i\alpha} - u_{j\alpha})(u_{k\beta} - u_{h\beta}) + \ldots
\]

Fit is performed on both Phonon and Strain-phonon terms.

- For a set \((TS)\) of configurations \((s)\) from DFT calculations, we fit with least squares method, the goal function is defined as:

\[
G[\lambda_p, TS] = \frac{1}{M_1} \sum_{s,\alpha,j} (F_{\alpha j}^{TS}(s) - F_{\alpha j}[\lambda_p](s))^2 + \frac{1}{M_2} \sum_{s,j} \Omega^2(s)(\sigma_j^{TS}(s) - \sigma_j[\lambda_p](s))^2
\]

- where \(\Omega(s) = (V(s)\sqrt{(N)})^{(-1/3)}\)

- The goal function has to satisfy \(\frac{\partial G[\lambda_p, TS]}{\partial \lambda_\mu} = 0 \ \forall \mu\) and \(\frac{\partial^2 G[\lambda_p, TS]}{\partial \lambda_\mu \partial \lambda_\nu} \geq 0 \ \forall \mu\nu\)

- We solve the system of p linear equations in order to get the set of coefficients \(\lambda_p\)
4. Fitting the Anharmonic part

```python
prt_model = 1
#
# Inputs for the fitted coefficients
#
fit_coeff = 1
fit_generateCoeff = 1
fit_rangePower = 3 4  # Range for the powers of the polynomial (default 3 to 4 )
fit_ncoeff = 7  # Number of coefficients to consider for the fit
fit_cutoff = 8  # Cutoff for the interactions
fit_anhaStrain = 0
fit_SPCoupling = 1

ts_option = 1
```

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4. Fitting the Anharmonic part

Example of CaTiO$_3$ cubic phase

- Mean Standard Deviation of the Energy with only Harmonic: 250.58 meV/f.u.
4. Fitting the Anharmonic part

Example of CaTiO$_3$ cubic phase

- Mean Standard Deviation of the Energy with only Harmonic: 250.58 meV/f.u.
- Mean Standard Deviation of the Energy with 1 Coef: 284.70 meV/f.u.
4. Fitting the Anharmonic part

Example of CaTiO$_3$ cubic phase

- Mean Standard Deviation of the Energy with only Harmonic: 250.58 meV/f.u.
4. Fitting the Anharmonic part

Example of CaTiO$_3$ cubic phase

- Mean Standard Deviation of the Energy with only Harmonic: 250.58 meV/f.u.
- Mean Standard Deviation of the Energy with 10 Coeffs: 12.75 meV/f.u.
4. Fitting the Anharmonic part

Example of CaTiO$_3$ cubic phase

- Mean Standard Deviation of the Energy with only Harmonic: 250.58 meV/f.u.
4. Fitting the Anharmonic part

Example of CaTiO$_3$ cubic phase

- Mean Standard Deviation of the Energy with only Harmonic: 250.58 meV/f.u.
- Mean Standard Deviation of the Energy with 50 Coeffs: 19.03 meV/f.u.
4. Fitting the Anharmonic part

Example of CaTiO$_3$ cubic phase

- Mean Standard Deviation of the Energy with only Harmonic: 250.58 meV/f.u.
- Mean Standard Deviation of the Energy with 100 Coeffs: 6.46 meV/f.u.
4. Fitting the Anharmonic part

Example of CaTiO$_3$ cubic phase

- Mean Standard Deviation of the Energy with only Harmonic: 250.58 meV/f.u.
- Mean Standard Deviation of the Energy with 175 Coeffs: 4.45 meV/f.u.
4. Fitting the Anharmonic part

Example of CaTiO$_3$ cubic phase

- Mean Standard Deviation of the Energy with only Harmonic: 250.58 meV/f.u.
- Mean Standard Deviation of the Energy with 175 Coeffs: 4.45 meV/f.u.
4. Fitting the Anharmonic part

Example of CaTiO$_3$ cubic phase

- Mean Standard Deviation of the Energy with only Harmonic: 250.58 meV/f.u.
- Mean Standard Deviation of the Energy with 175 Coeffs: 4.45 meV/f.u.
5. Additional care

Bounding the potential

- If the highest order is odd
- If the highest order is even and the coefficient negative

⇒ The potential might be unstable !!
- Add artificial physics with maths to bound the process.

→ See M. Schmitt presentation.
5. Additional care

Analyzing the results
$q(Agate)$

- Visualize the trajectory
- Perform all “MD” analysis (PDF, T, P, V, …)
- Extract phonons at finite temperature (with a-TDEP see F. Bottin talk)
- Project on modes and follow phase transitions
6. Conclusion

Lattice part

- Multibinit is able to make interface between first principles calculations and mesoscopic simulations for "any" system
- Automatic construction of the models with harmonic and anharmonic contributions from first principles
- Automatic bound process
- Tool able to run dynamics (Monte Carlo or Molecular dynamics)
- Good tools for result analysis and post-processing of data ((q)Agate)
- New ionmov in abinit to generate the training set
6. Conclusion

Miscellaneous

- Spin potential available (X. He talk)
- Spin dynamics available (X. He Talk)
- Spin-lattice coupling (N. Helbig)
- Effective Hamiltonian WIP (W. Lafargue-dit-Hauret poster)
- Coupling with electronic potential (M. Schmitt and previous talks)
- Common data structure for ease of use and interfacing
6. Conclusion

Thank You!

- ULiège: Marcus Schmitt, He Xu, Nicole Helbig, Fabio Ricci, Matthieu Verstraete, Eric Bousquet, Philippe Ghosez
- UCLouvain: Gian-Marco Rignanese, Xavier Gonze
- Others: Alexandre Martin, Sergeï Prokhorenko, Andrés Camilo García Castro

Interactions also with:
- USantander: Javier Junquera and Pablo García-Fernández
- LIST: Jorge Íñiguez