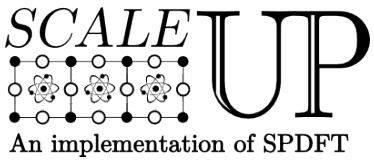

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Construction of complex Effective Lattice Models with MULTIBINIT and Electron-Lattice Couplings combining MULTIBINIT & SCALE UP

Michael Marcus SCHMITT

Jordan BIEDER, Fabio RICCI, Pablo GARCIA-FERNANDEZ, Javier JUNQUERA, and Philippe GHOSEZ

9th international ABINIT developer workshop

20-22nd May 2019 - Louvain-la-Neuve, Belgium

1. Complex Effective Lattice Models

THE LATTICE MODEL IN MULTIBINIT

$$E_{tot}(\mathbf{u},\eta) = E_0(\mathbf{r_0},0) + E(\mathbf{u},\eta)$$

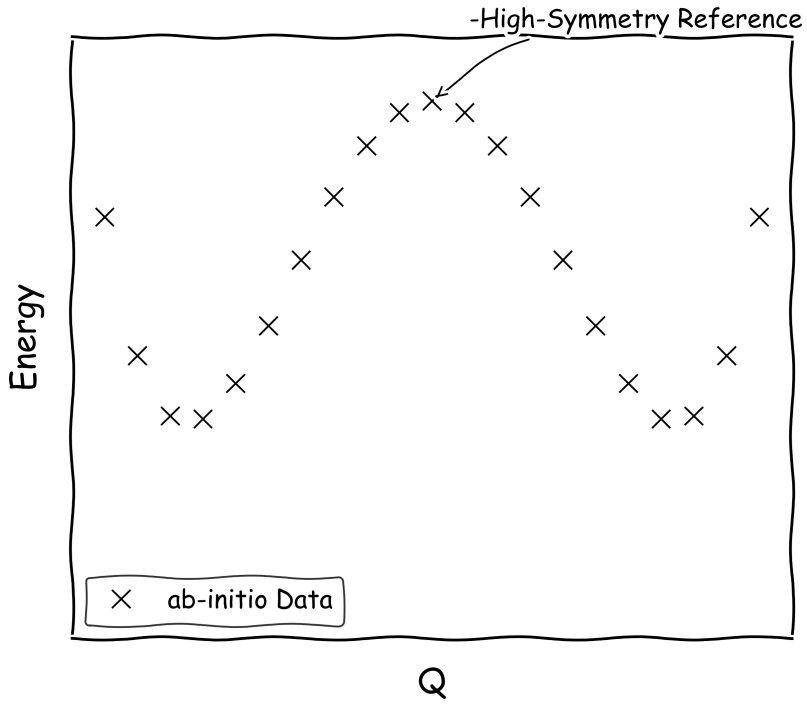
$$E(u,\eta) = E^{phonon}(u) + E^{strain}(\eta) + E^{strain-phonon}(u,\eta)$$

$$E^{ph}(\mathbf{u}) = \sum_{ijkh\alpha\beta} K^{(2)}_{ijkh\alpha\beta}(u_{i\alpha}-u_{j\alpha})(u_{k\beta}-u_{h\beta}) + \sum_{ikhrt\alpha\beta\gamma} K^{(3)}_{ikhrt\alpha\beta\gamma}(u_{i\alpha}-u_{j\alpha}) \times (u_{k\beta}-u_{h\beta})(u_{r\gamma}-u_{t\gamma})\dots$$

$$E^{s}(\eta) = \sum_{ab} C_{ab}\eta_a\eta_b$$

$$E^{s-ph}(\{\mathbf{u}\},\eta) = \sum_a \sum_{ij\alpha} \Lambda^{(1,1)}_{aij\alpha}\eta_a(u_{i\alpha}-u_{j\alpha}) + \sum_a \sum_{ijhk\alpha\beta} \Lambda^{(1,2)}_{aijhk\alpha\beta}\eta_a(u_{i\alpha}-u_{j\alpha}) \times (u_{k\beta}-u_{h\beta})\dots$$

Transform Ab-Initio Data into Polynomial Description



Q: A direction of displacements $(\mathbf{u}, \eta)$

Harmonic part extracted from DFPT - Higher order Fitted

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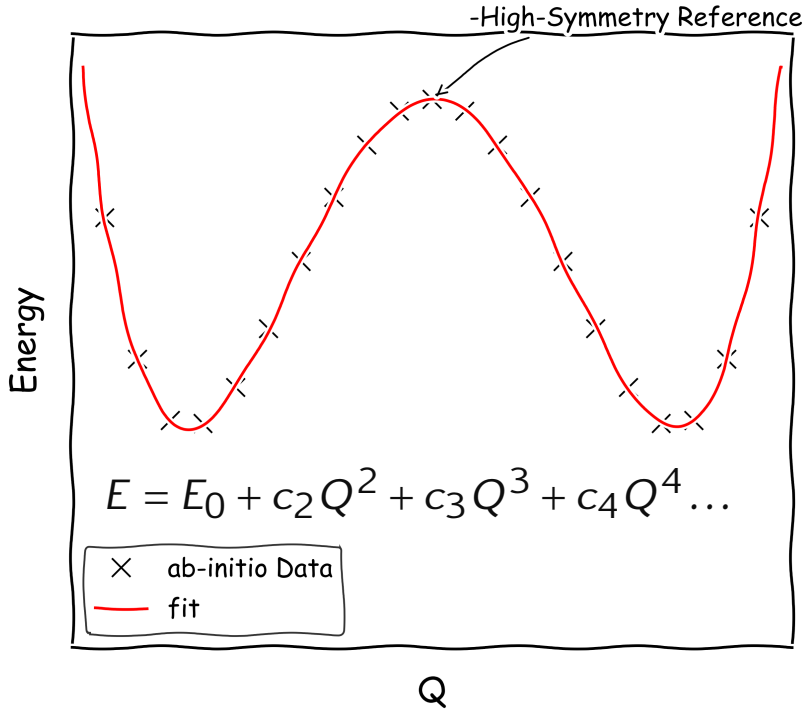

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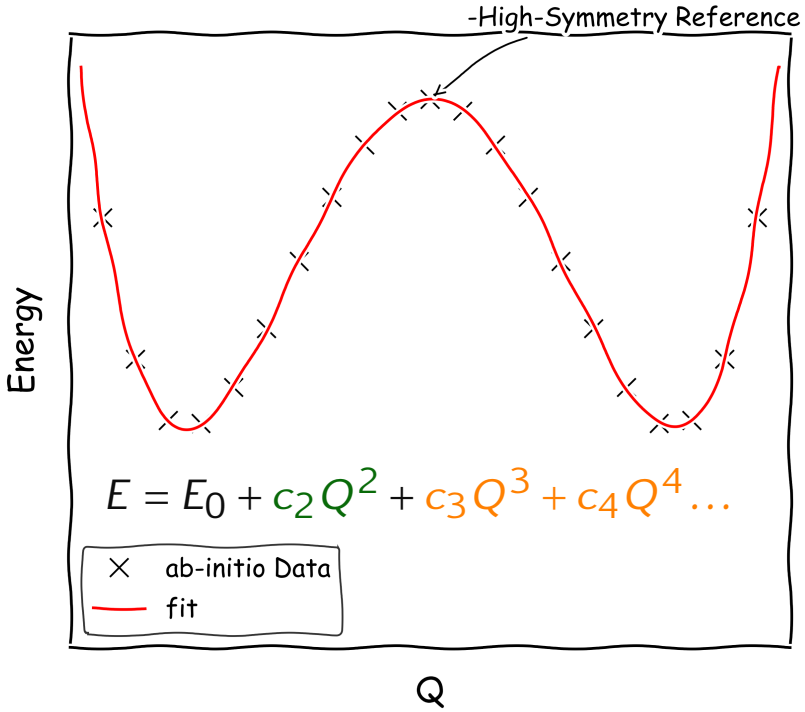

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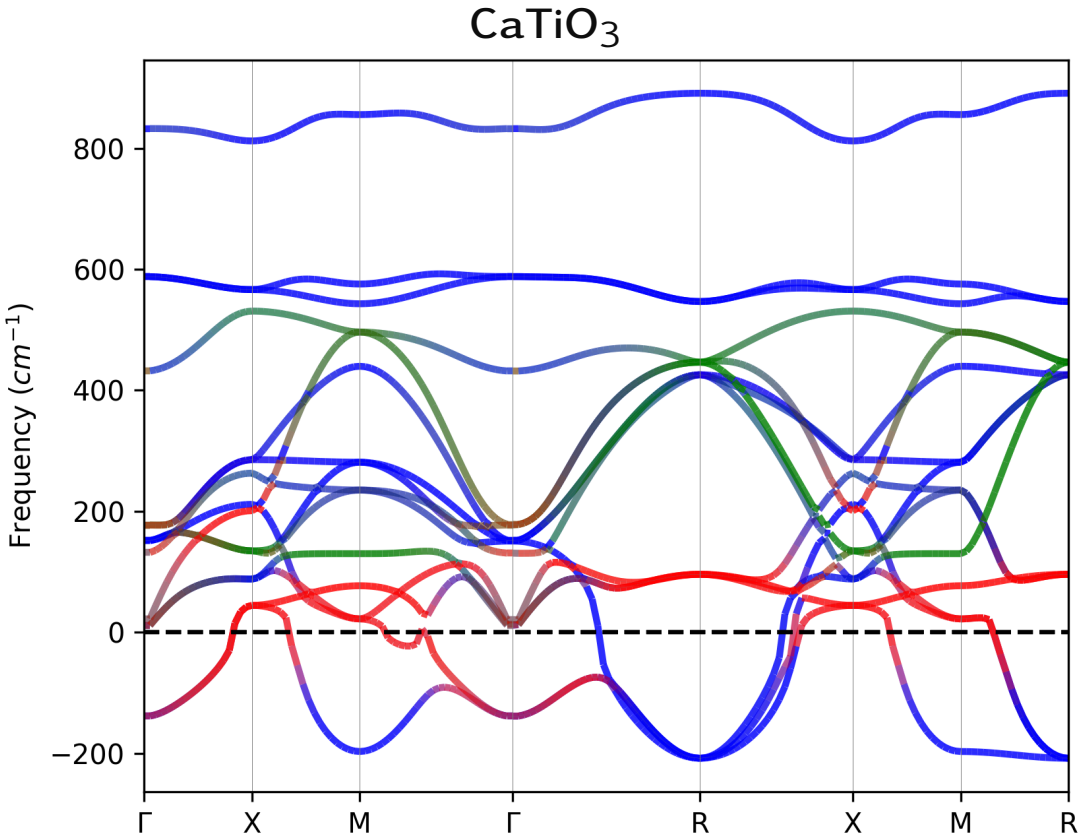
Real Materials Might Have Many Instabilities and Complex Ground-State Structures



Ground-State Structure *Pnma*: Composed of 5 modes and 2 strains

Largest displacement about 0.4 Å ≈ 10% of LC

Competing Phases $R\bar{3}c$,*I*4/*mcm*, *P*4/*mbm*, *Cmcm*

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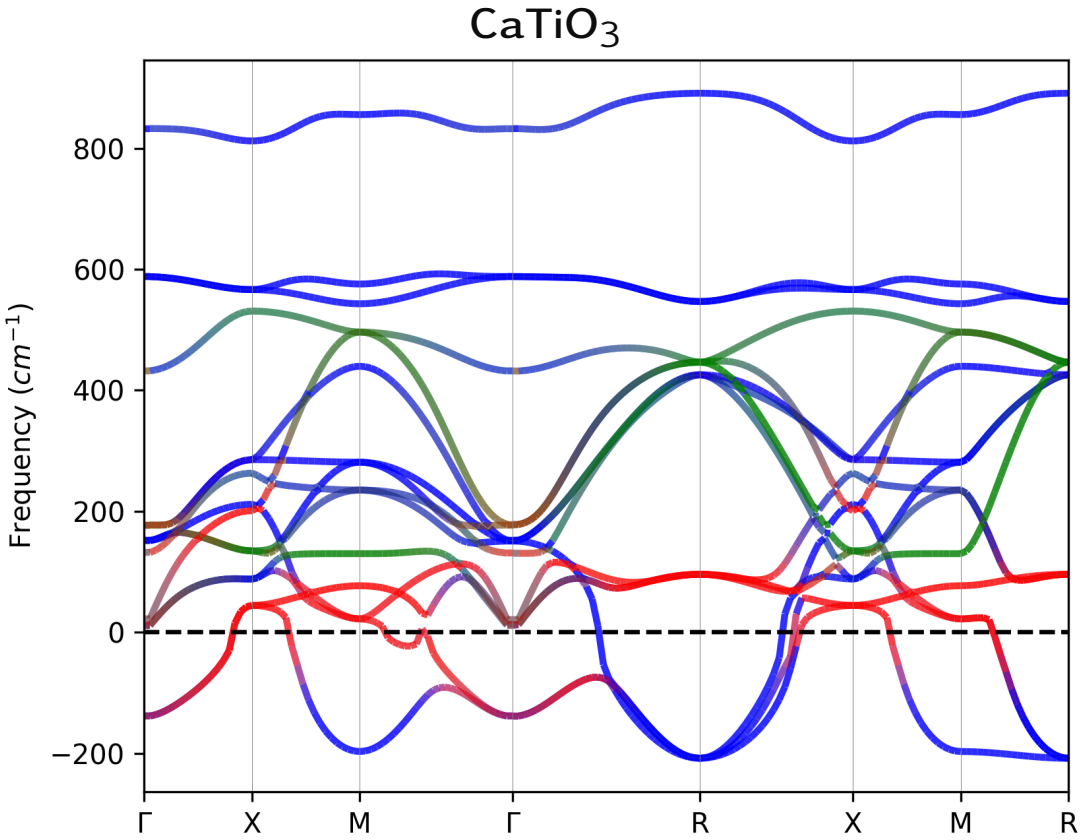

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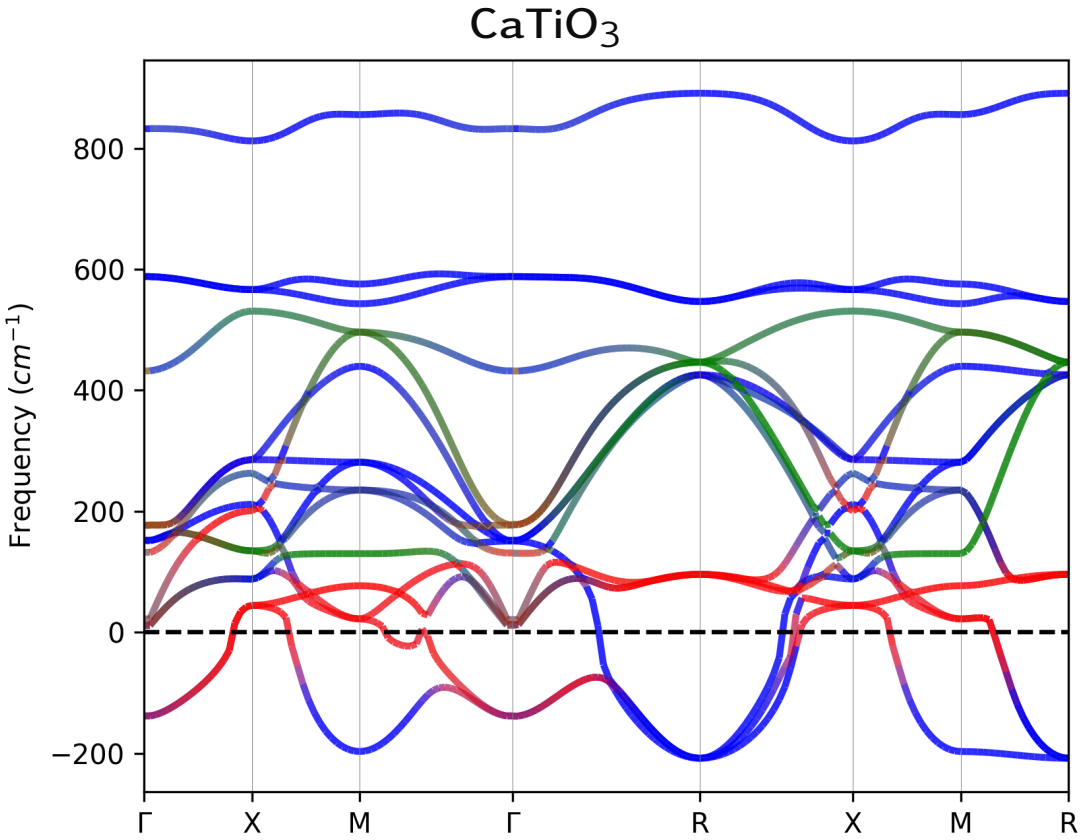

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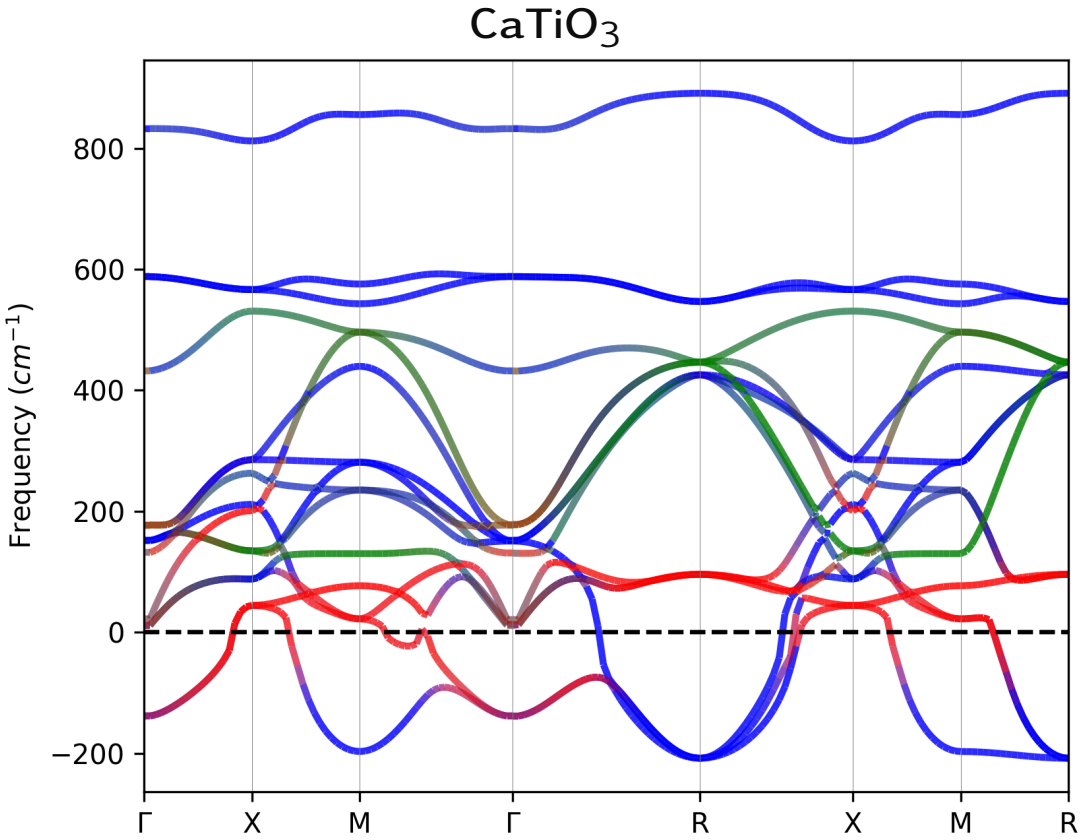

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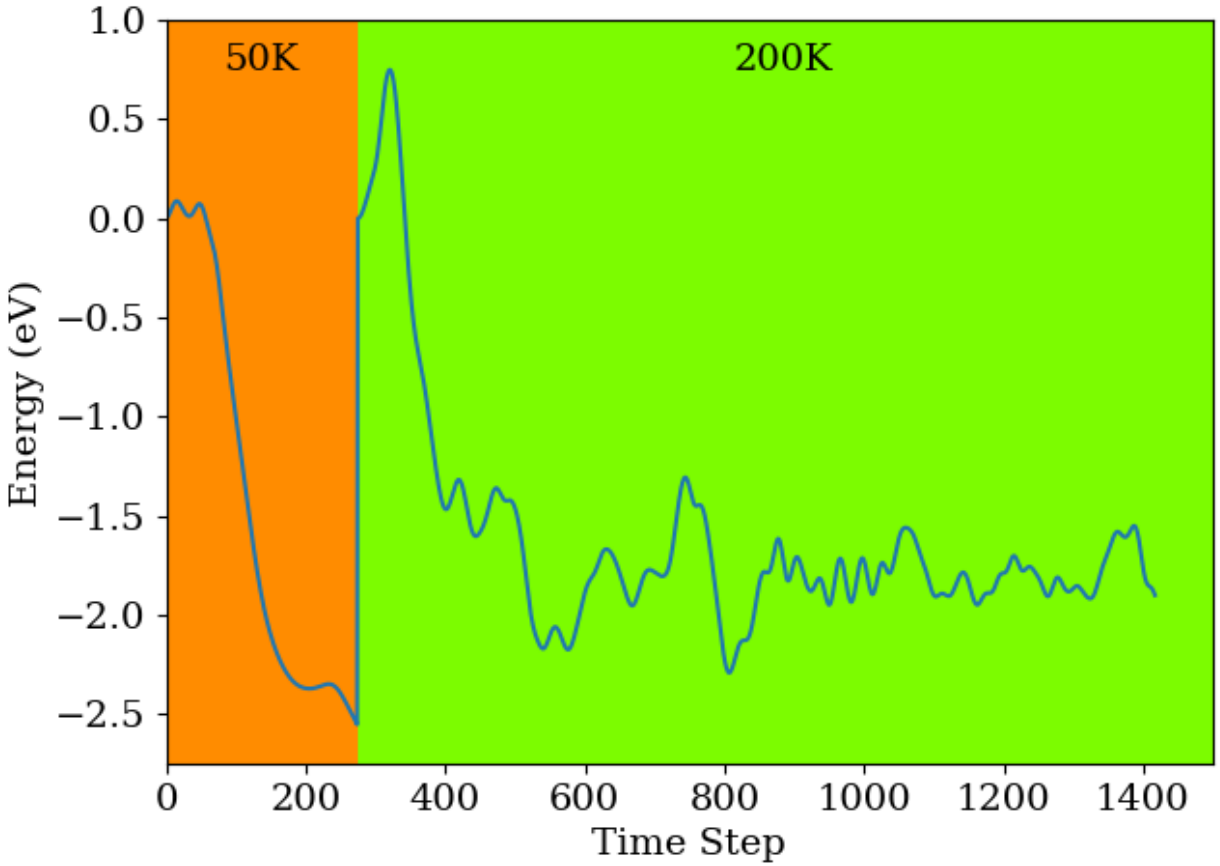
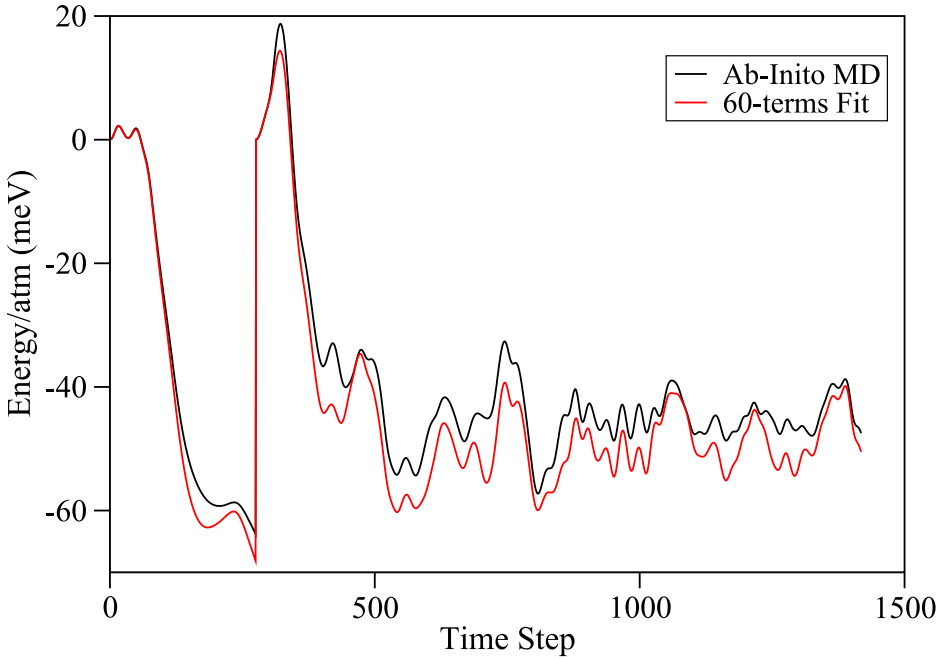
Use Ab-Initio Molecular Dynamics to Sample Instable Paths



A First Free Fit Using Multibinit




```
Mean Standard Deviation values of the effective-potential (meV/atm):
  Energy          :   4.0803665397763584E+00
Goal function values of the effective.potential
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  Forces+Stresses :   2.4466967954928562E-02
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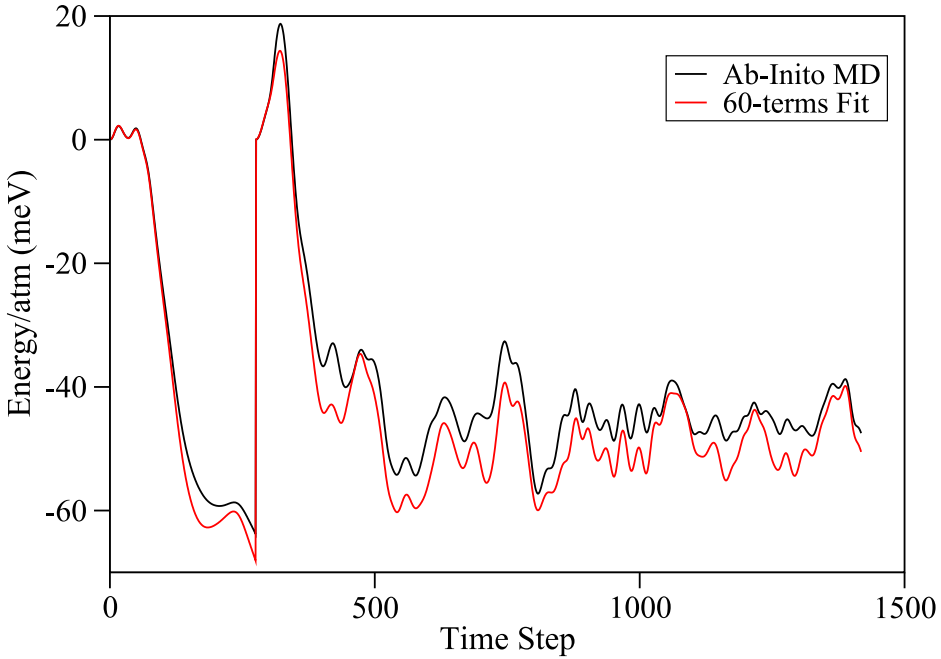

At T=50K Model goes to the *Pnma*-phase

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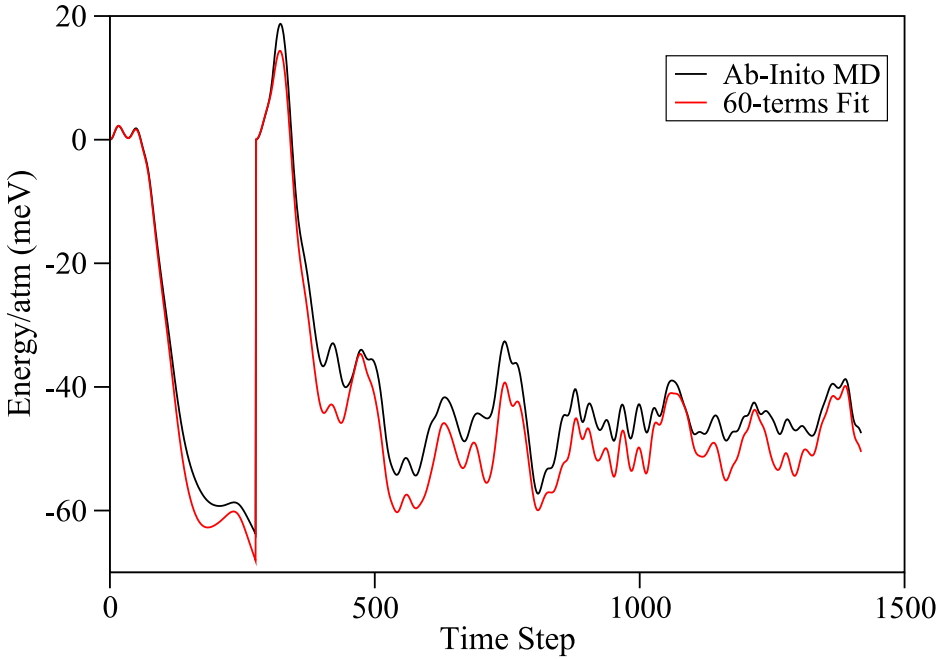

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5000-steps,40-atoms ≈ 70s on 4 cores

```
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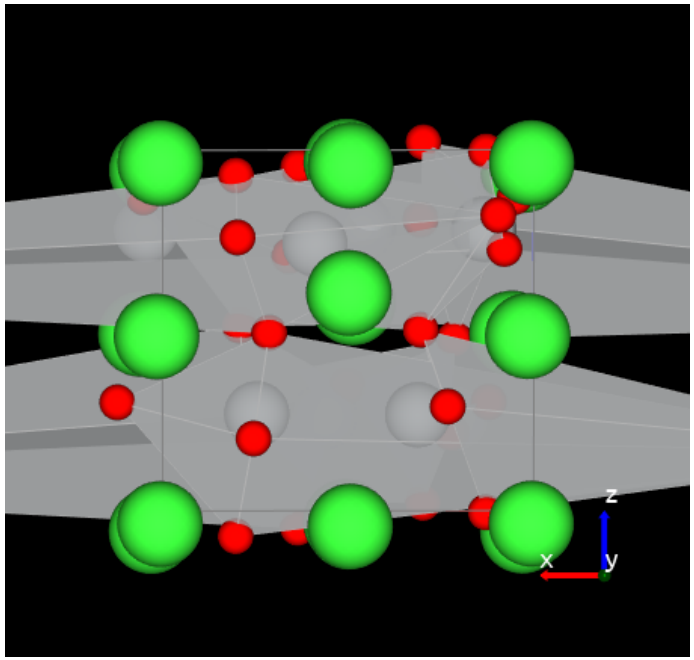
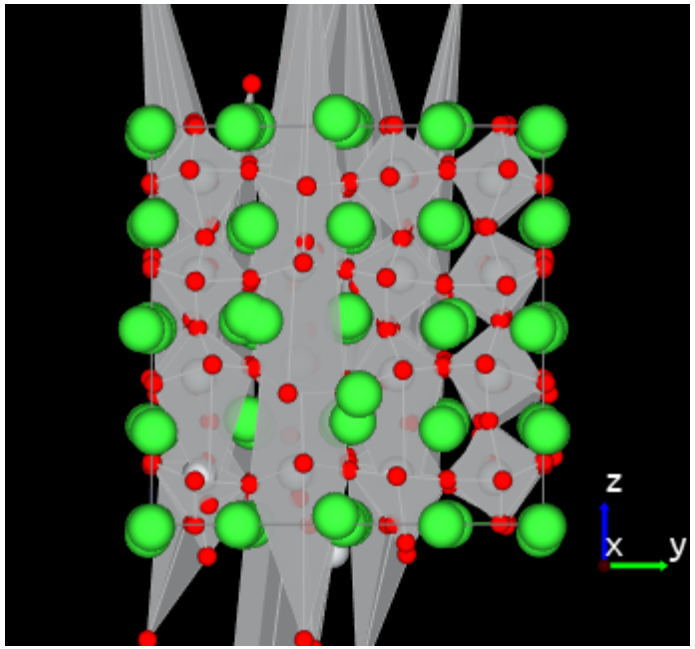
```

"Boundedness" is a Big Problem

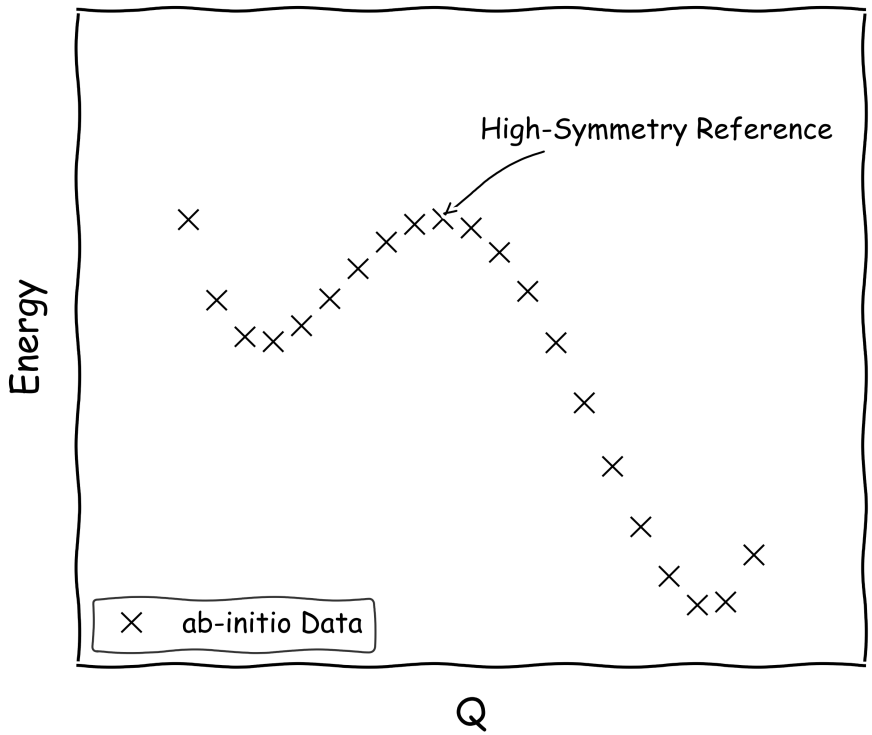
T = 300K



ncell = 4x4x4 = 320 atoms



"UnBoundedness" - Negative Divergence in The Effective Potential



Appears if highest order term in Q is odd or even with negative coeffcient

Add higher order terms to bound in direction Q! How to keep precision?

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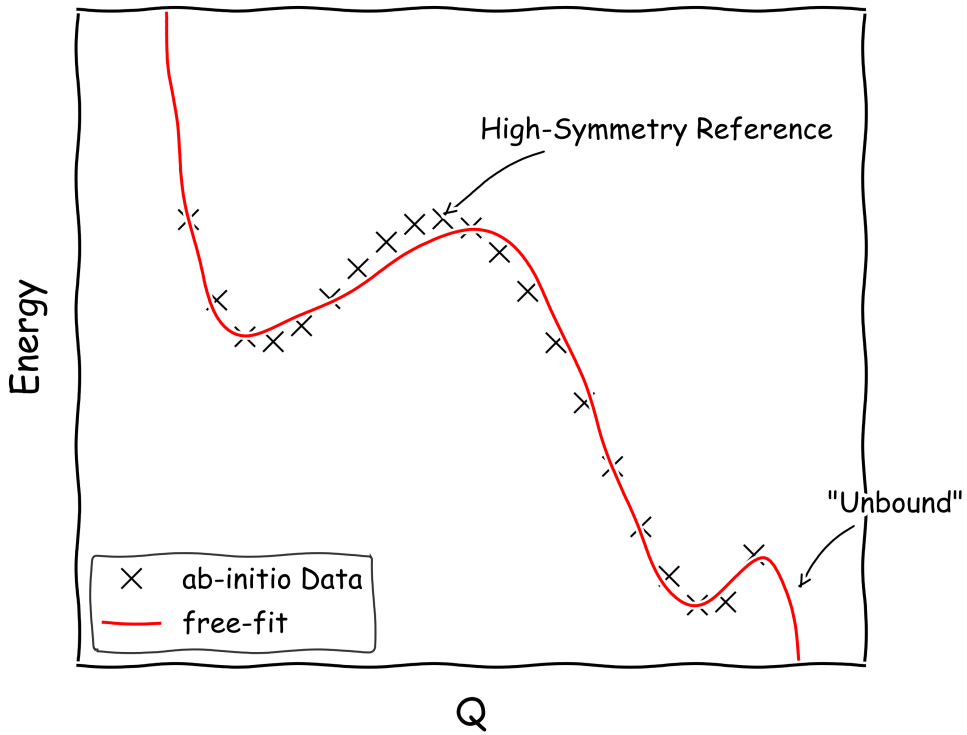

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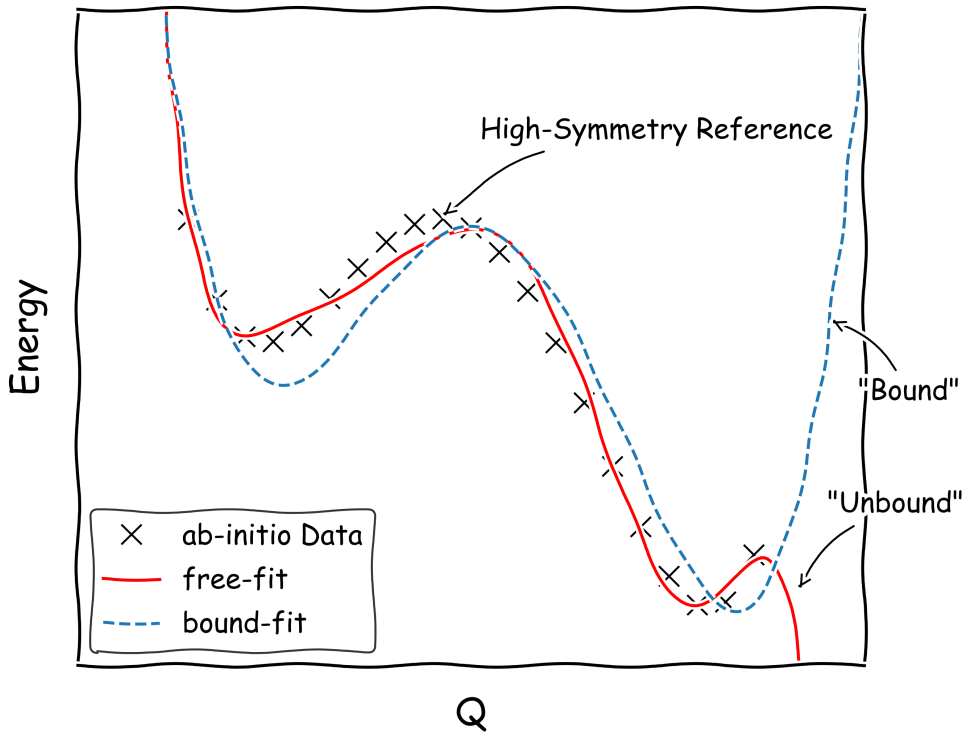

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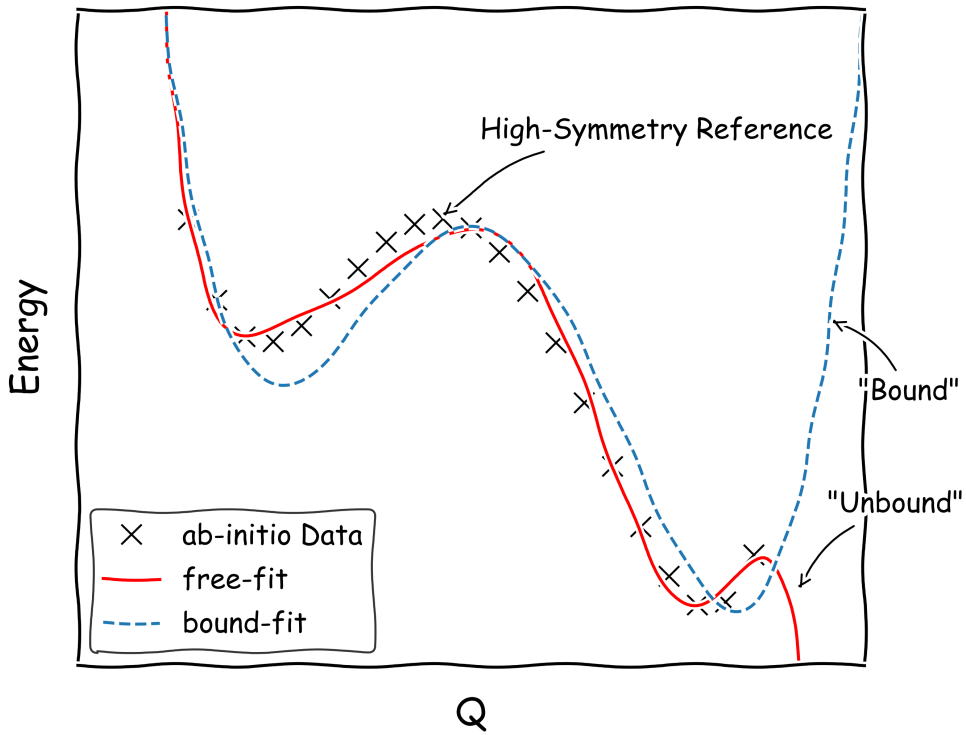

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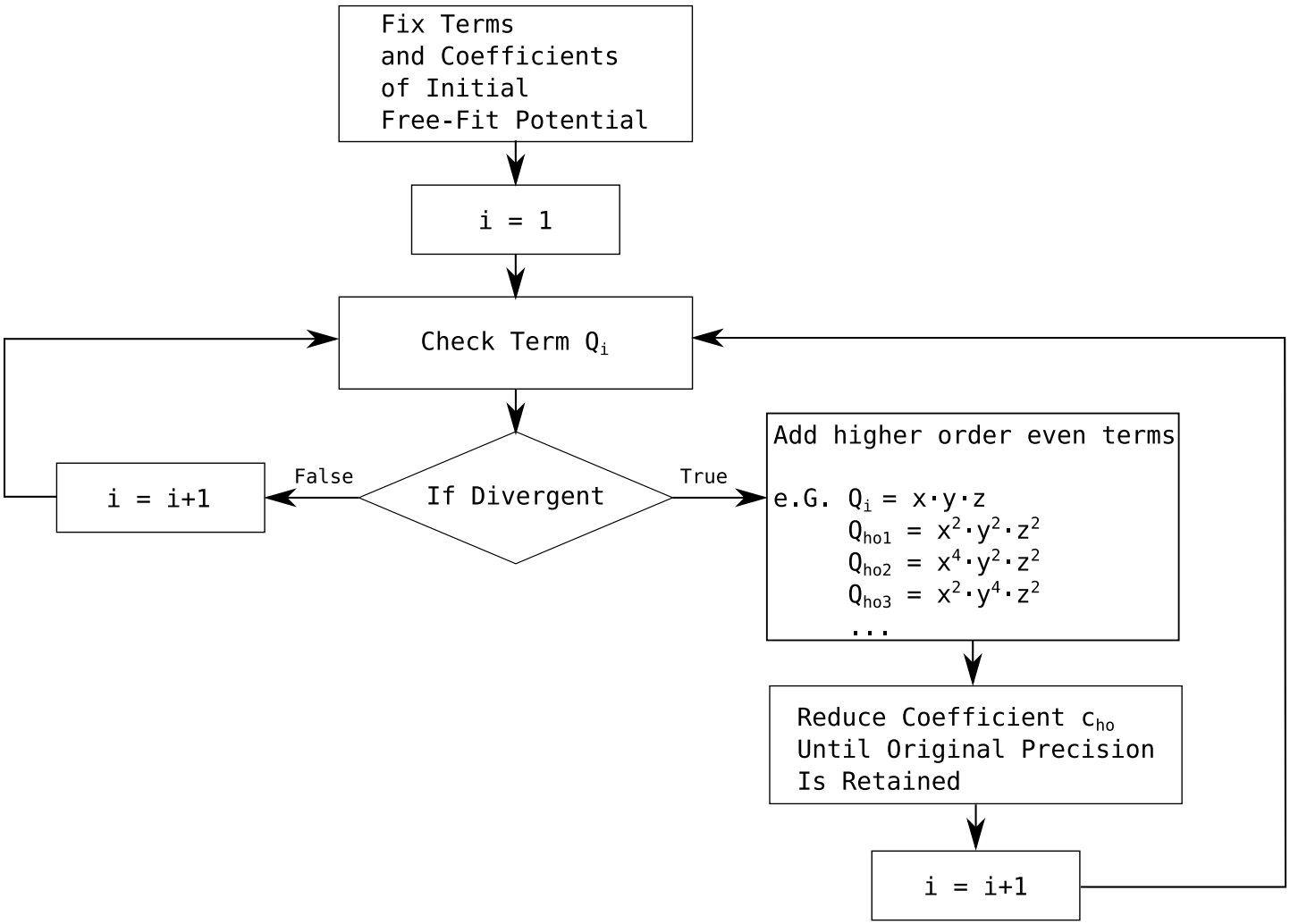
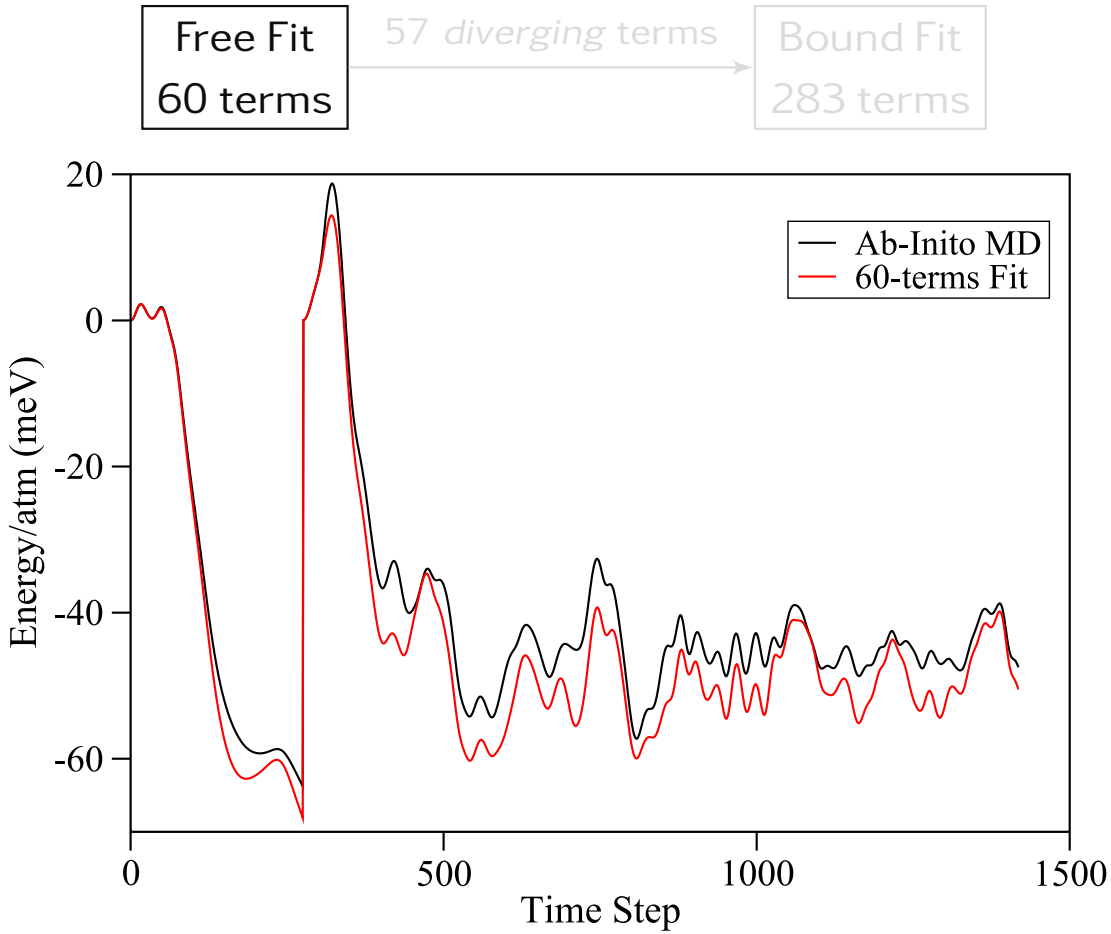
A Simple Algorithm to Impose Boundedness



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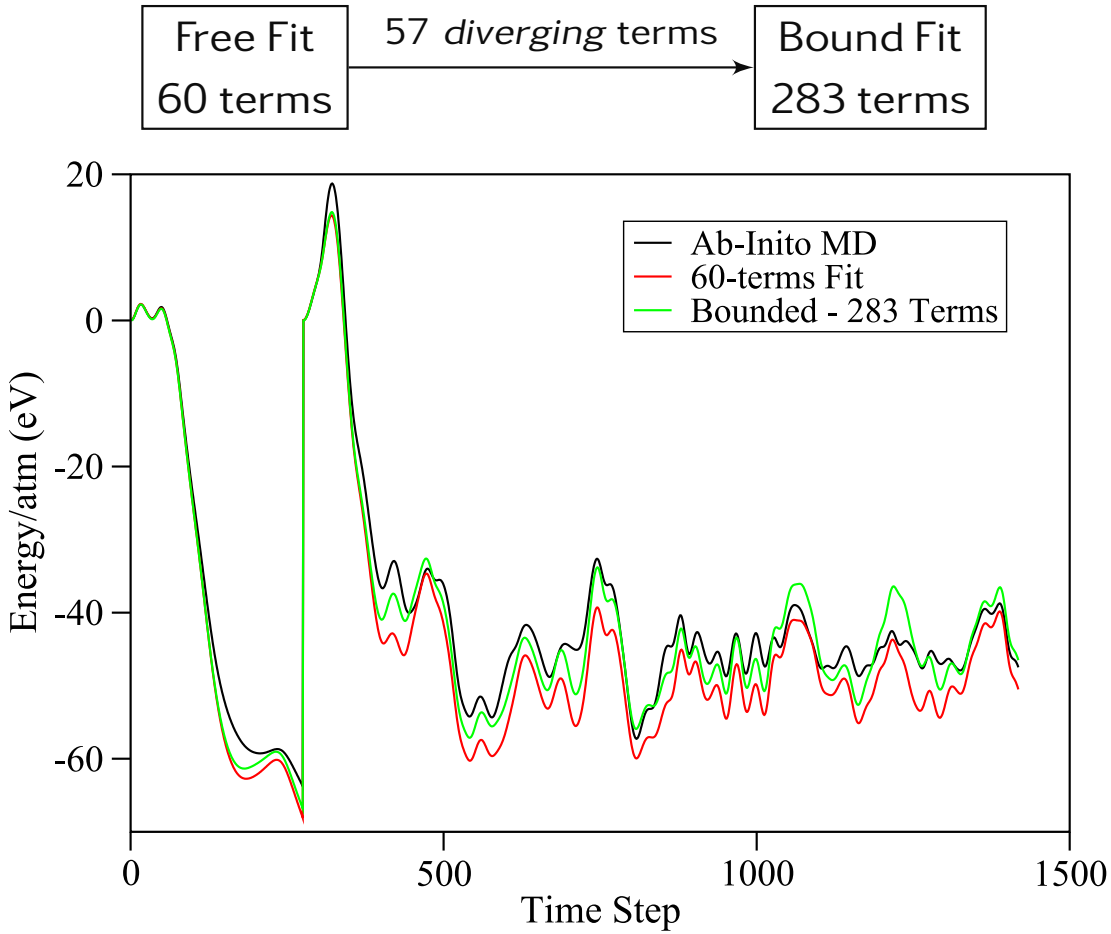


```
Mean Standard Deviation values of the effective-potential (meV/atm):
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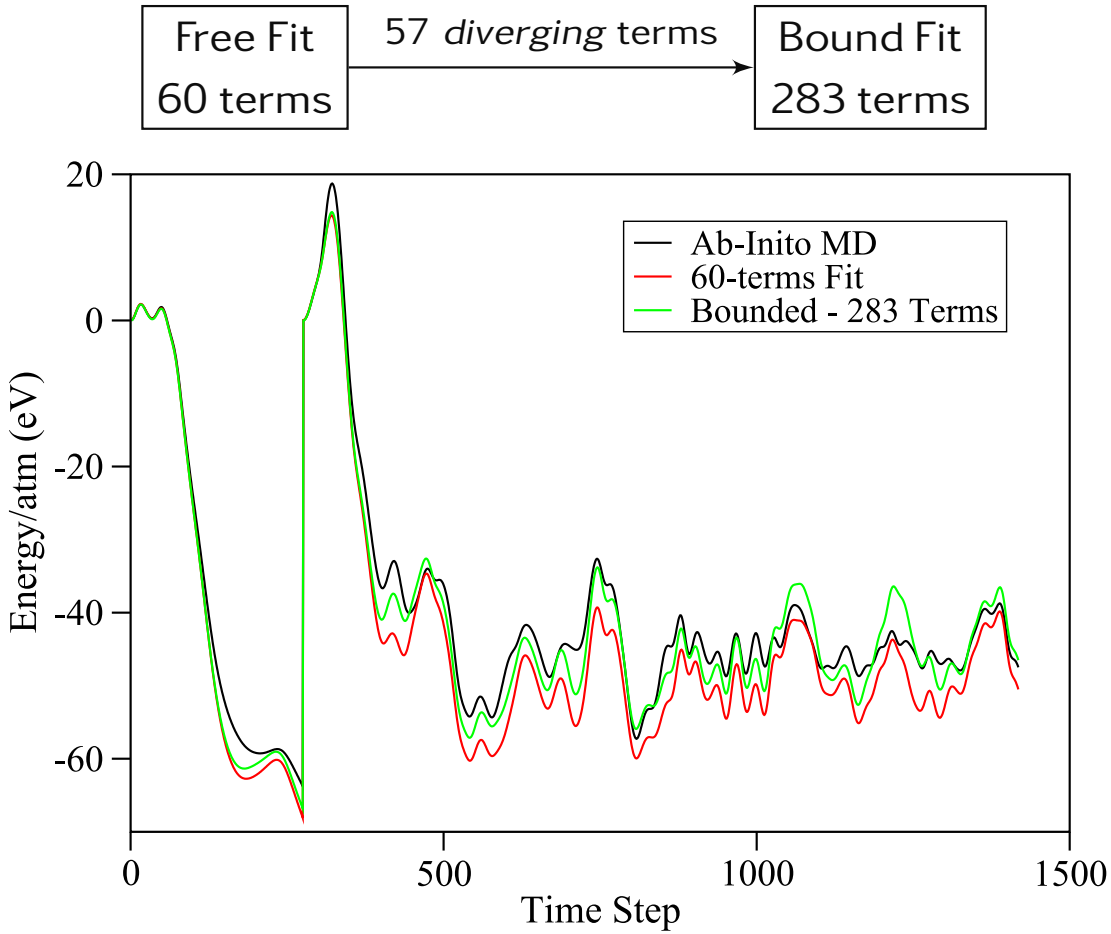
```

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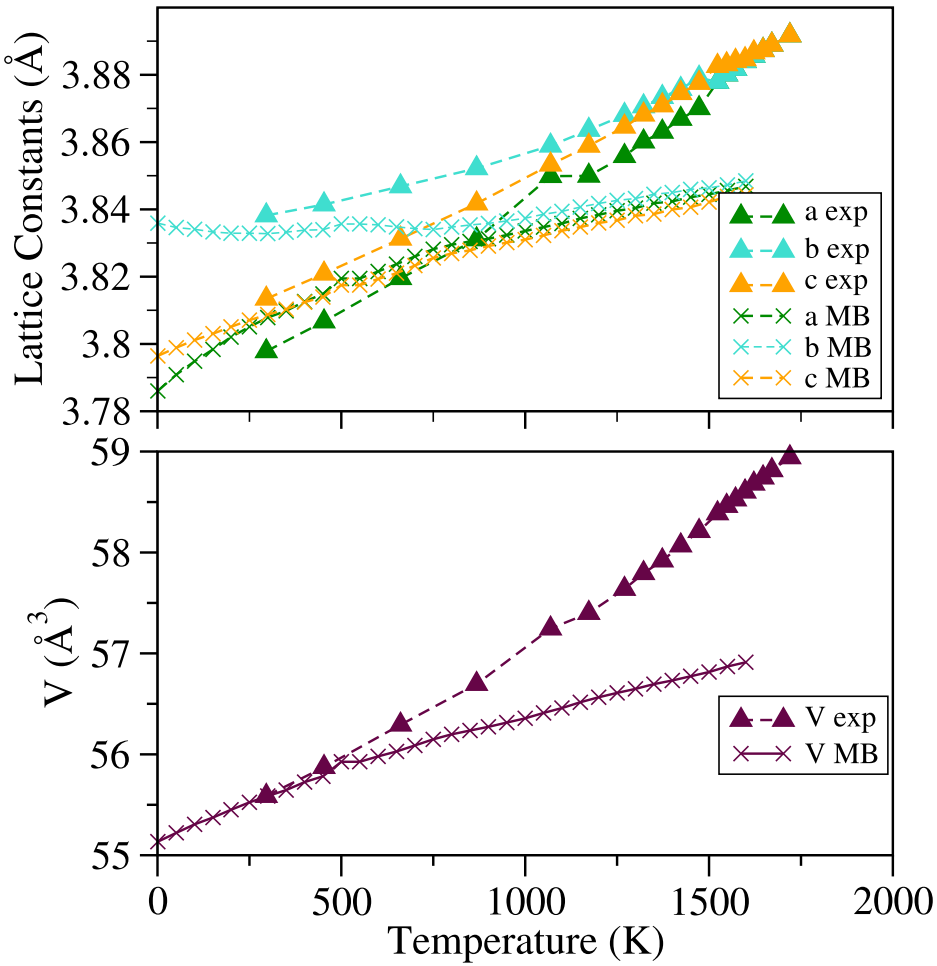
```

The model is bound

16x16x16 cells, 20480 atoms

6000-steps per temperature

96-cores ≈ 1h15min per temperature



Yashima, M. & Ali, R., Solid State Ionics, 2009, **180**, 120 - 126

2. Electron-Lattice Coupling Using MULTIBINIT and SCALE-UP

The Information about the electronic states are hidden in the lattice effective potential parameters

$$E_{tot}(\mathbf{u},\eta) = E_0(\mathbf{r_0},0) + E(\mathbf{u},\eta)$$

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Reintroduce some electronic states of interest with SCALE-UP

$$E_{tot}(\mathbf{u},\eta) = E_0(\mathbf{r_0},0)) + E(\mathbf{u},\eta) + E_{el}(\mathbf{u},\eta)$$

$$E_{el}(\mathbf{u},\eta) = \sum_{ab} D^U_{ab}\gamma_{ab}(\mathbf{u},\eta) + 1/2\sum_{ab}\sum_{a'b'} D^U_{ab}D^U_{a'b'}U_{aba'b'} - D^I_{ab}D^I_{a'b'}I_{aba'b'}$$

With the central quantity: $D_{ab} = d_{ab} - d^{(0)}_{ab}$

And the electron-lattice coupling expressed in

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$$+ \sum_{ikhrt\alpha\beta\gamma} K_{i} \ldots u_{i\alpha} - u_{j\alpha})$$

$$\times (u_{k\beta} - u_{l} \ldots$$

Access

- Electronic Structure at Finite T
- Electronic Structure of Large Scale Objects
- $D_{ab} \neq 0$: Magnetic States, Polarons, Excitons

Reint… …E-UP

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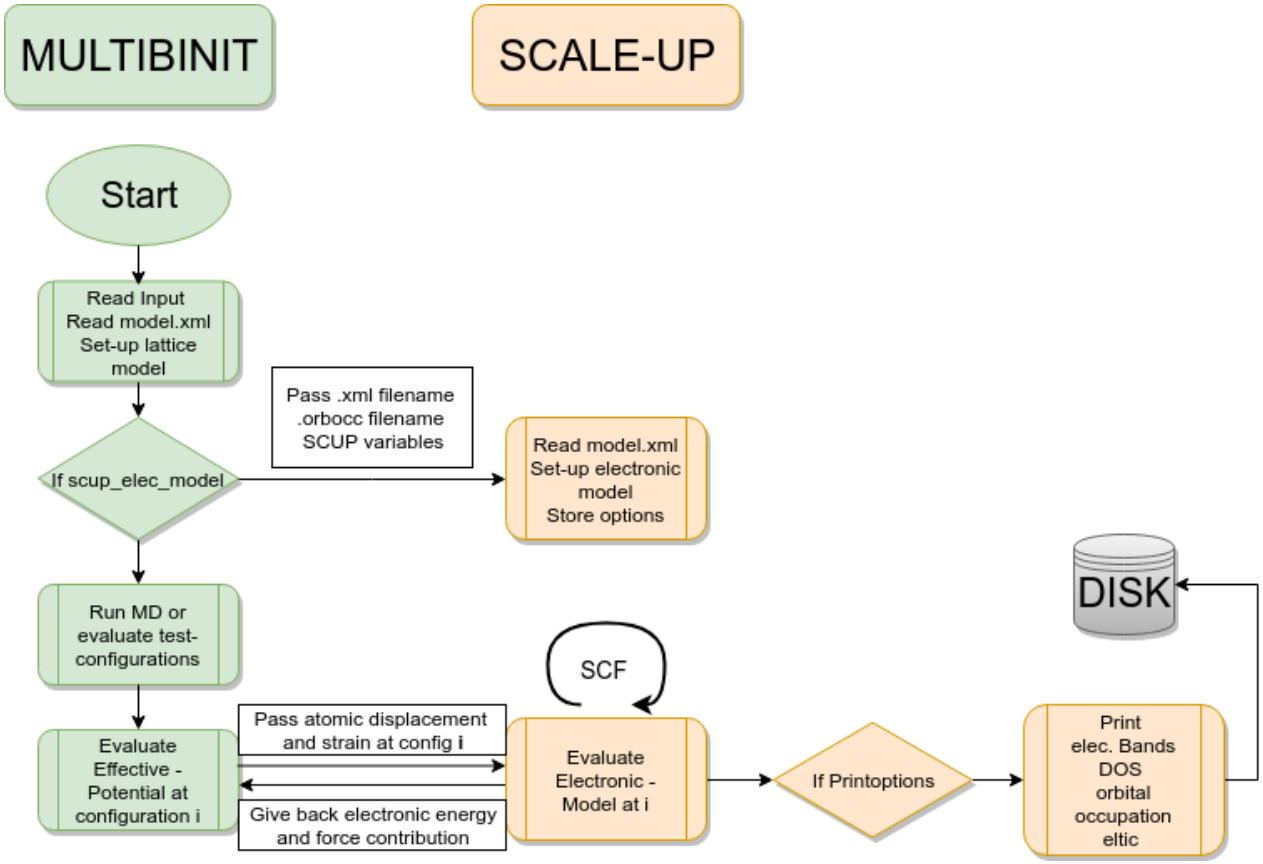
THE MULTIBINIT - SCALE-UP INTERFACE

Multibinit incorporates SCALE-UP as a library

```
FC_LIBS="-L/path/to/scaleup/build/src/.libs/ -lscaleup"
```

Lattice and Electronic Model share the same modelfile .xml



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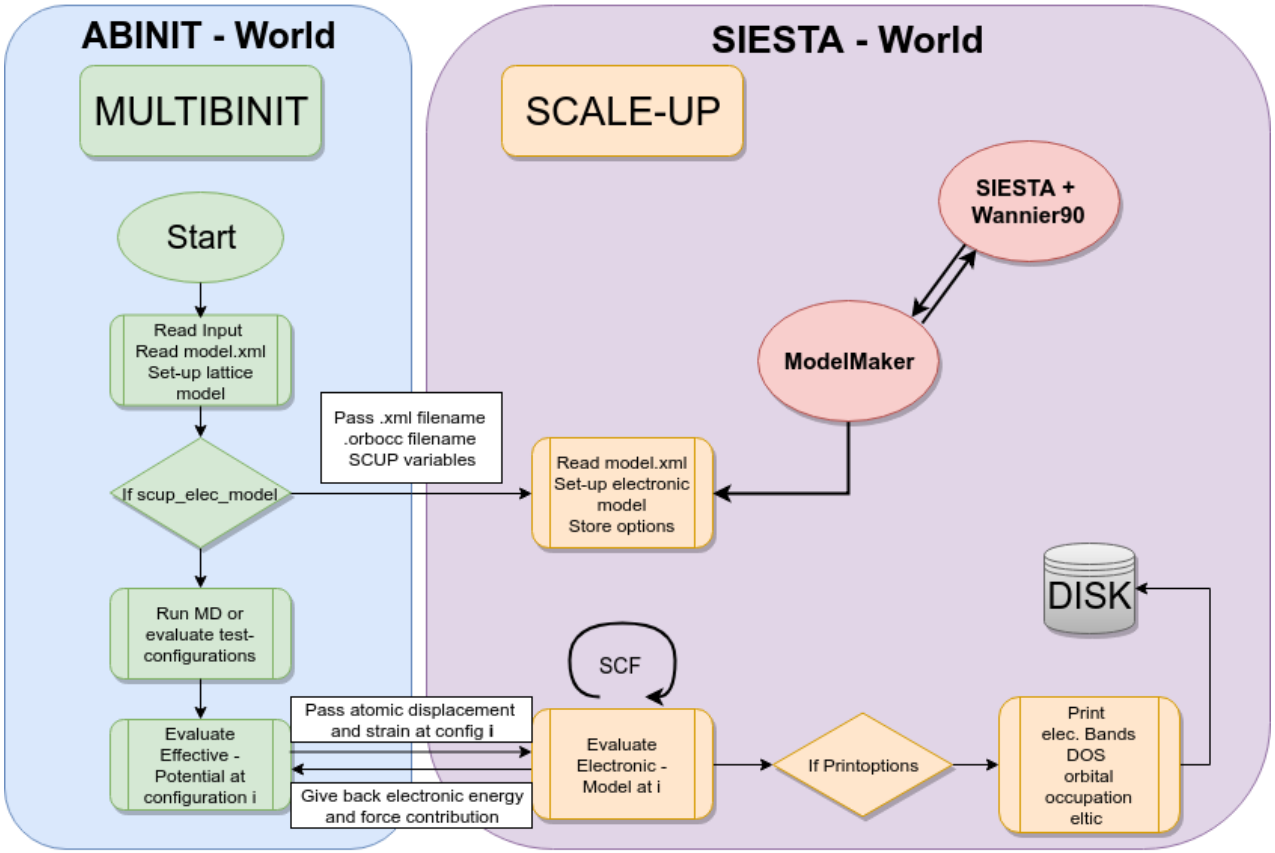
```

Lattice and Electronic Model share the same modelfile .xml



Code Licensing/Distribution ?!

THE MULTIBINIT - SCALE-UP INTERFACE

The SCALE-UP variables are parsed with their one parser

```
abinit/src/78_effpot/m_scup_dataset.F90
```

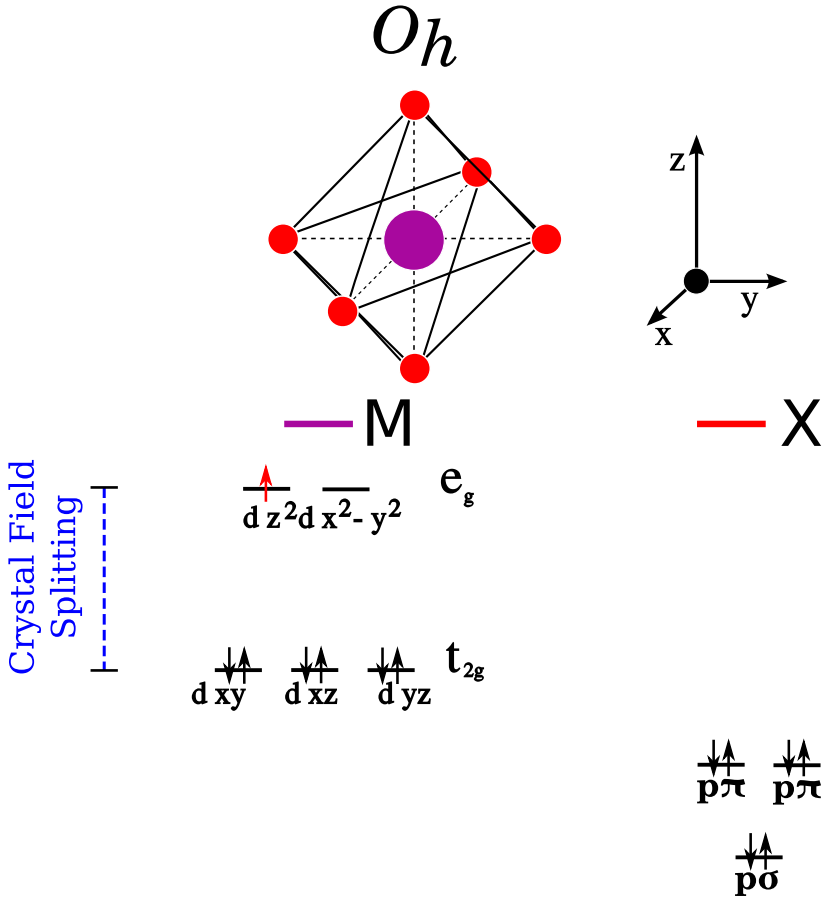
And stored in a separate datatype

```
type scup_dtset_type
!Integer
 integer :: scup_nspeck
 integer :: scup_ndivsm
 integer :: scup_printniter
!Logicals
 logical :: scup_elec_model
 logical :: scup_initorbocc
 logical :: scup_ismagnetic
 logical :: scup_istddft
 logical :: scup_printbands
 logical :: scup_printeigv
 logical :: scup_printeltic
 logical :: scup_printgeom
 logical :: scup_printorbocc
!Real
 real*8   :: scup_tcharge
!Integer Array
 integer :: scup_ksamp(3)
!Real Array
 real(dp),allocatable :: scup_speck(:,:)
!Kpath Type
 type(kpath_t) :: scup_kpath
 end type scup_dtset_type
```

A first model using electron-lattice coupling

Classical Problem of cooperative Jahn-Teller Effect in Perovskites

Corner shared transition metal octahedra with double-degenerate electronic state



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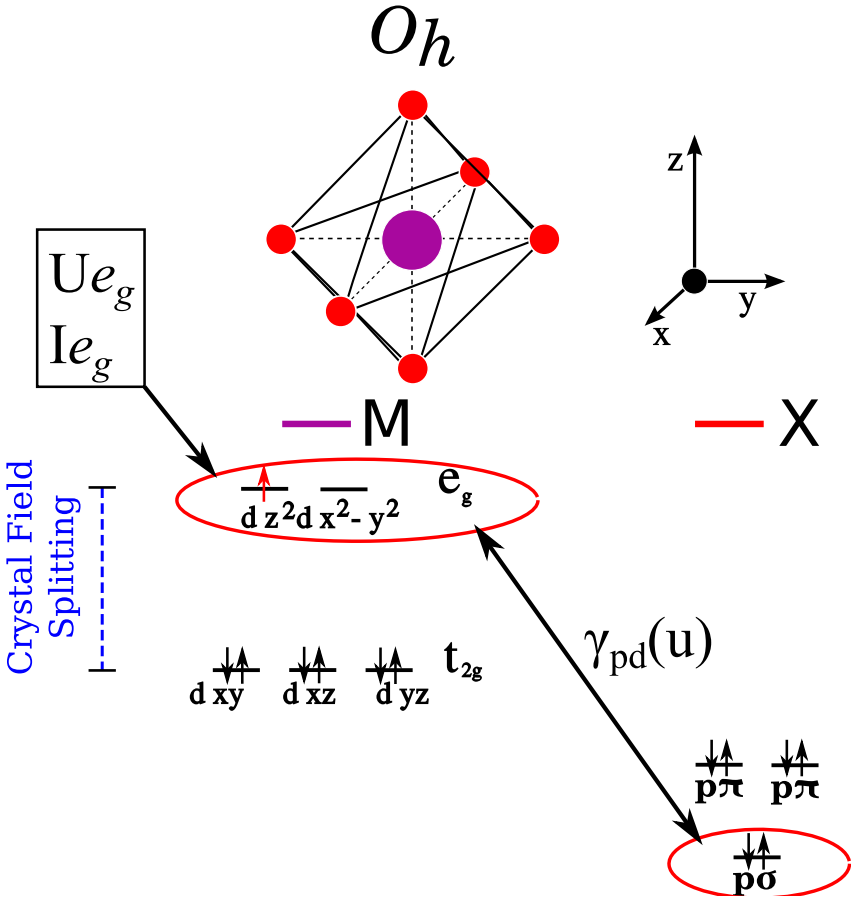
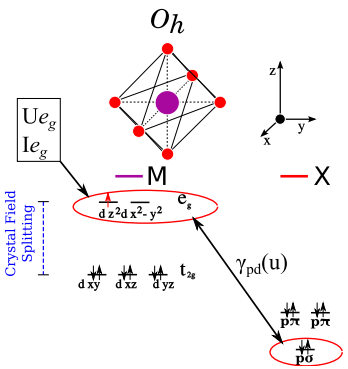


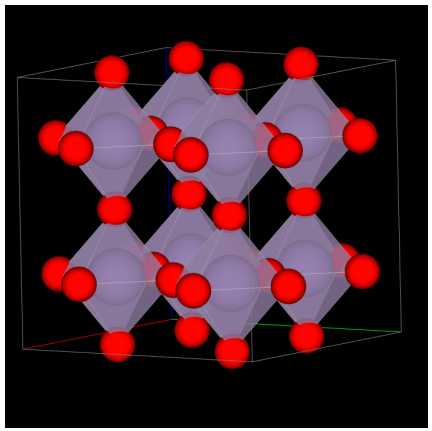
A first model using electron-lattice coupling

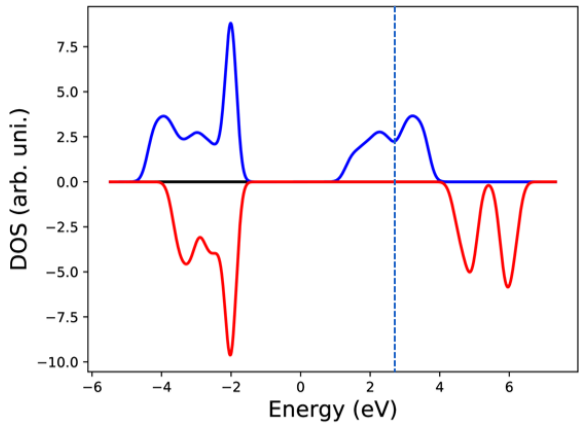
Electron-Lattice Coupling - Investigate Band-Structure and DOS

$$U_{e_g} = 3eV, I_{e_g} = 1.5eV, \gamma_{pd} = 1.5eV$$

Cubic

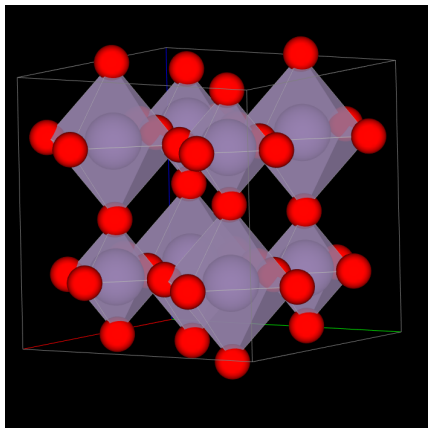


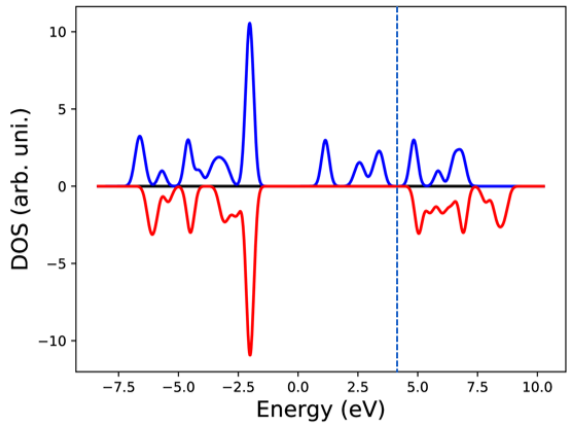




Spin-up

Q_1^R





Spin-Down

Conclusions

- Complex Lattice Effective Potentials
  - A new bound algorithm to facilitate automatic generation of effective lattice potentials
  - $CaTiO_3$ model describes correctly temperature development in the Ground-State Phase
- MULTIBINIT + SCALE-UP Interface
  - Coupled effective lattice-electronic models open exciting possibilities

Outlook

Challenges for the MULIBINIT-SCUP Project

1. Code Licensing and Distribution

Should MB-SCUP interface move to the trunk ?

2. Testing

Have a special builder on the test-farm ?

3. Further integration of Datastructure

SCUP input/output in the abinit _HIST.nc Format ?

Thank you for your Attention!

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