

Crystal Structure Prediction using a genetic algorithm

Phases of TiO_2

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◎Crystal Structure Prediction widget:

- General fields – see below
- I/O tab – next slide
- Genetic Algorithm tab – after next slide
- Optimization – next slide

Bandstructure Analyzer...

Compare Data...

Complex Bandstructure Analyzer...

Crystal Structure Prediction Scripter...

Deformation Potential Analyzer...

Effective Bandstructure Analyzer...

File

Chemical Formula

There will be 6 atoms per unit cell.

External pressure GPa

Initial volume Å³

Genetic Algorithm Optimization **I/O**

Random number seed

Initial population log prefix

Crystal structure prediction log prefix

☒ Write population

◎General fields

- Type (TiO2)2 or Ti2O4
- Leave external pressure at 0
- Initial volume is calculated automatically

Setting up the calculation



⦿ I/O tab:

- Leave at default values

The screenshot shows the 'I/O' tab selected in the software interface. The 'Chemical Formula' is set to (TiO2)2, with a note 'There will be 6 atoms per unit cell.' Below this, 'External pressure' is 0 GPa and 'Initial volume' is 51.57 Å³. The 'I/O' tab contains the following settings: 'Random number seed' is set to 'Automatic', 'Initial population log prefix' is 'initial_population_', 'Crystal structure prediction log prefix' is 'generation_', and the 'Write population' checkbox is checked. A red rectangular box highlights the entire I/O tab area.

⦿ Optimization tab:

- Leave at default values

The screenshot shows the 'Optimization' tab selected in the software interface. The 'Chemical Formula' is set to (TiO2)2, with a note 'There will be 6 atoms per unit cell.' Below this, 'External pressure' is 0 GPa and 'Initial volume' is 51.57 Å³. The 'Optimization' tab contains the following settings: 'Force tolerance' is 0.01 eV/Å, 'Pressure tolerance' is 0.1 GPa, 'Maximum number of steps' is 1000, and 'Maximum step length' is 0.2 Å. A blue rectangular box highlights the entire Optimization tab area.



⦿ Genetic Algorithm:

- *Population size*: Number of individual crystal structures in each generation.
- *Number of generations*: The number of iterations the algorithm will go through.
- *Selection pressure*: Higher values will assign more weight to structures with a higher fitness when applying genetic operators.
- *Number of elites*: Number of individuals used for creating the next generation. All individuals with lower fitness are discarded.
- *Number to promote*: Number of crystal structures which will be copied to the next generation without change.

File

Chemical Formula

There will be 6 atoms per unit cell.

External pressure GPa

Initial volume Å³

Genetic Algorithm Optimization I/O

Population Size

Number of generations

Selection pressure

Number of elites

Number to promote

Genetic Operators

Heredity weight

Permutation weight

Mutation weight

Mutation lattice strain

➔



Genetic Operators:

- *Heredity weight*: The unnormalized probability that an individual in the new generation is created by the Heredity operator, combining two structures from the previous generation.
- *Permutation weight*: The unnormalized probability of applying the Permutation operator, which exchanges the positions of two atoms of different elements.
- *Mutation weight*: The unnormalized probability of applying the Mutation operator, which distorts the cell with a symmetric strain matrix, with strain values drawn from a Gaussian distribution with standard deviation of *Mutation lattice strain*.

File

Chemical Formula

There will be 6 atoms per unit cell.

External pressure GPa

Initial volume Å³

Genetic Algorithm Optimization I/O

Population Size

Number of generations

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Genetic Operators

Heredity weight

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Mutation weight

Mutation lattice strain

➔

Setting up the calculation - Calculator



- ⦿ Set up a TiO₂ structure in the Builder
- ⦿ Set up an ATK-Classical calculator
 - Set it to the Pedone_2006Fe2 parameter set.
- ⦿ Copy the calculator to the script from the CSP widget

The screenshot shows the 'Calculators' dialog box with the 'ATK-Classical' option selected. The 'Potential Settings' section shows the 'Parameter set' as 'Pedone_2006Fe2'. The 'Literature References' section contains a citation for A. Pedone et al. (2006). The 'Additional Info' section has checkboxes for 'Save' and 'Print', both of which are checked. The 'IO' section shows the 'File' as 'Rutile.nc' and an empty 'Label' field. The 'Calculator settings' section shows the 'Potential' tab selected. The 'Estimate Memory Usage' button is visible at the bottom left, and the 'OK' button is at the bottom right.

Calculators

- ☐ ATK-DFT
- ☐ ATK-SE: Extended Hückel
- ☐ ATK-SE: Slater-Koster
- ☒ ATK-Classical
- ☐ Abinit
- ☐ FHI-aims

Potential Settings

Parameter set:

Literature References

A. Pedone and G. Malavasi and M. Menziani and A. Cormack and U. Segre, *A new self-consistent empirical interatomic potential model for oxides, silicates and silica-based glasses*, J. Phys. Chem. B, 110, pp. 11780-11795, 2006.

Additional Info

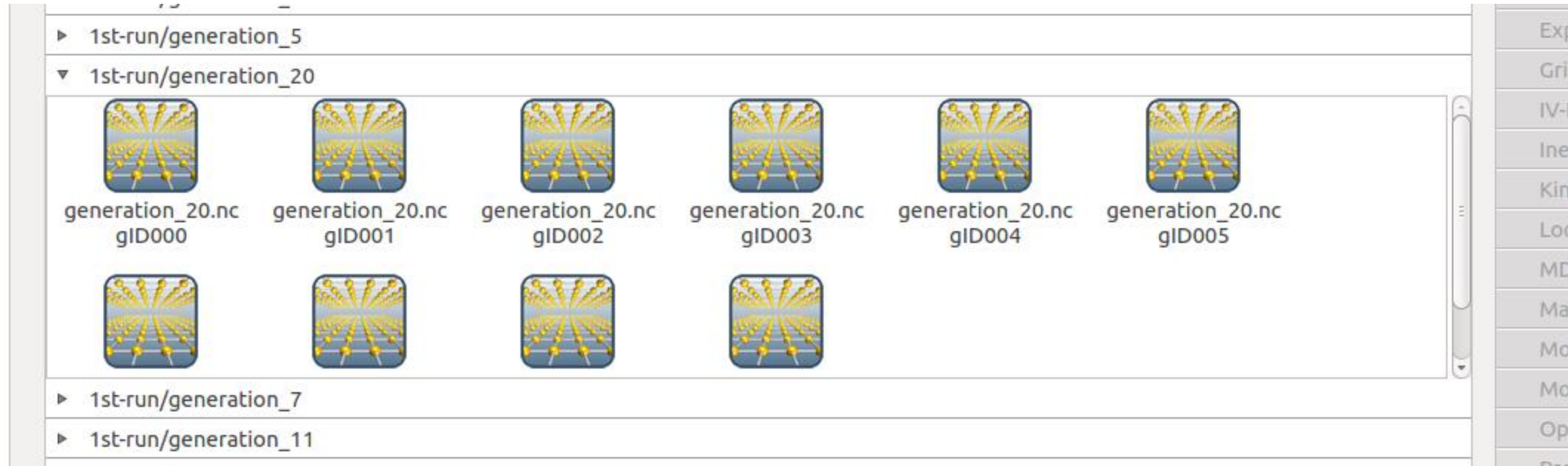
IO

☒ Save ☒ Print

File: ... Label:



- ◎ All BulkConfigurations are available in .nc-files for each generation



Thank You!

Quantum
Wise

