Crystal Structure Prediction using a genetic algorithm

Phases of TiO$_2$

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Setting up the calculation

Crystal Structure Prediction widget:
- General fields – see below
- I/O tab – next slide
- Genetic Algorithm tab – after next slide
- Optimization – next slide

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

- **Optimization tab:**
  - Leave at default values
Setting up the calculation

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.
Setting up the calculation

- **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*. 
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.
- **Niching**: Duplicate individuals are discarded.

- **Fitness**: The negative of the enthalpy.

- **History**: The sequence of operations leading to this crystal structure.

Symmetries P4_2/mnm and I4_1/amd are consistent with rutile and anatase.
Results

- All BulkConfigurations are available in .nc-files for each generation.
Thank You!

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