Crystal Structure Prediction using a genetic algorithm

Phases of TiO_2

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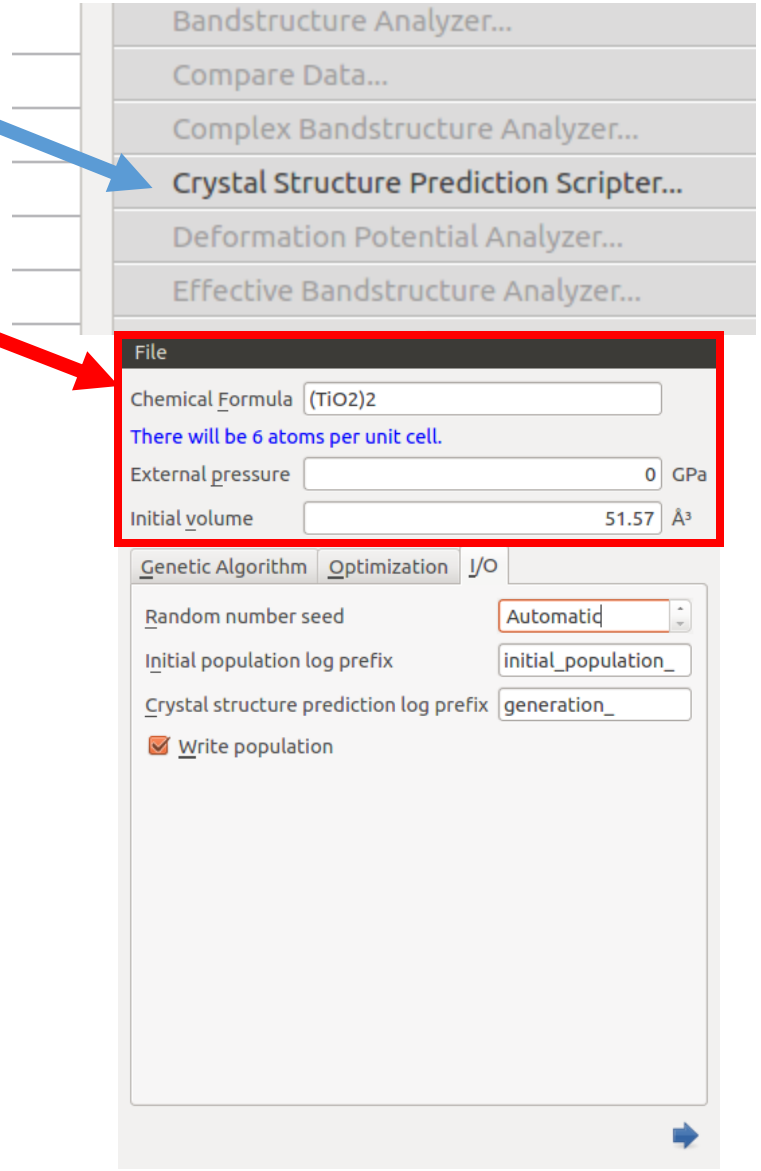
Setting up the calculation

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

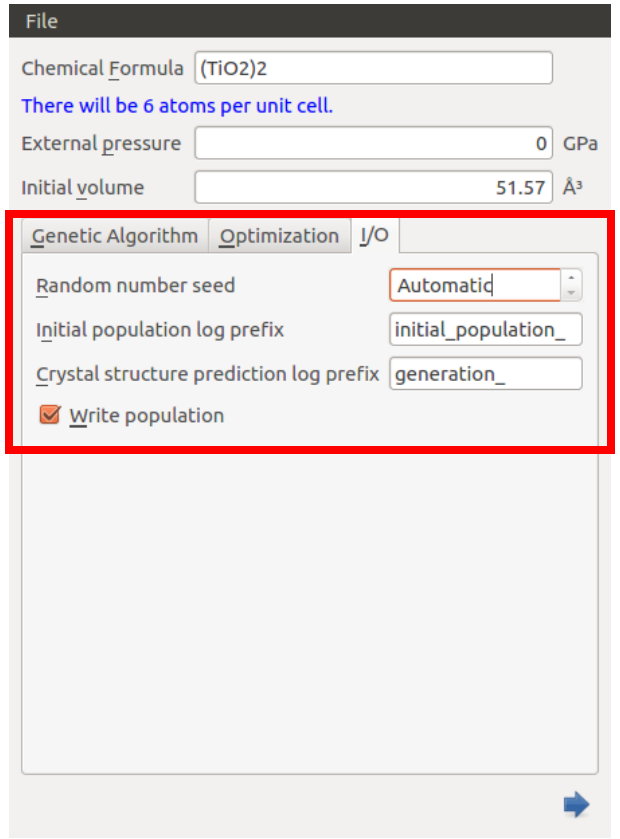


- General fields
  - Type (TiO2)2 or Ti2O4
  - Leave external pressure at 0
  - Initial volume is calculated automatically

Setting up the calculation

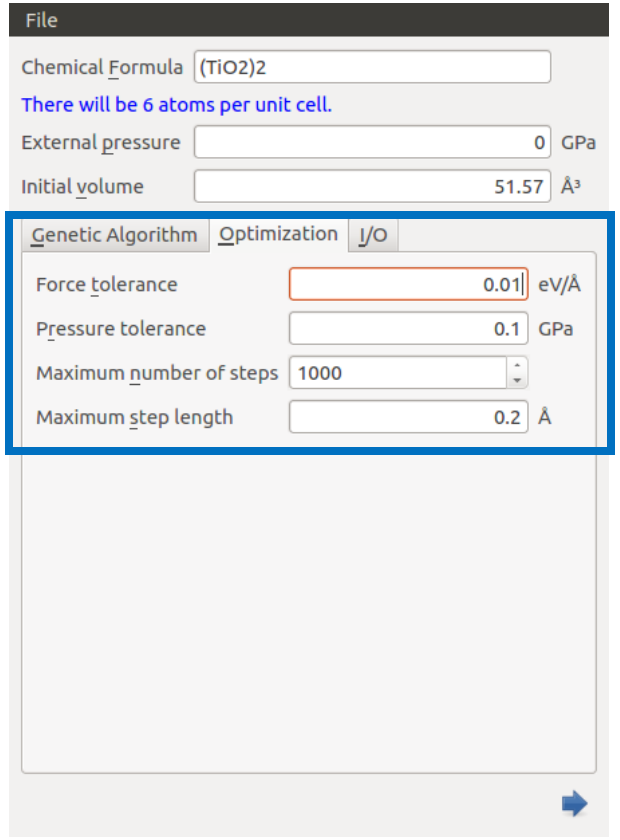
⊙I/O tab:

- Leave at default values



⊙Optimization tab:

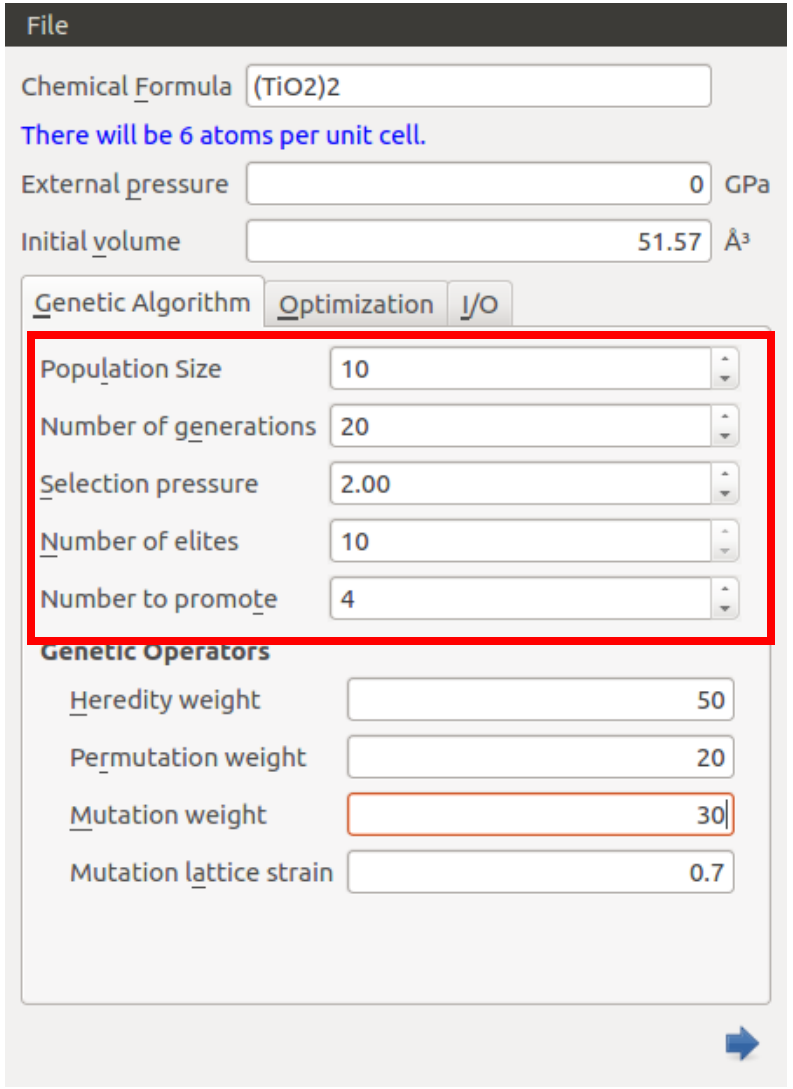
- Leave at default values



Setting up the calculation

⊙Genetic Algorithm:

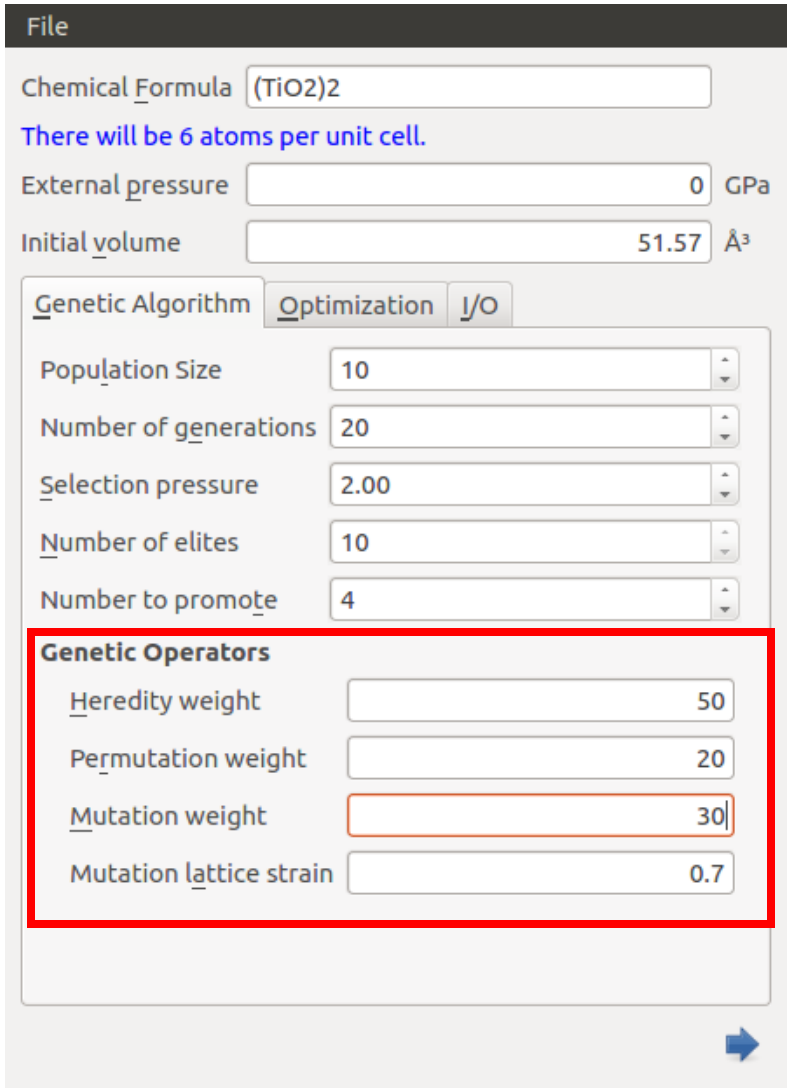
- *Population size*: Number of individual crystal structures in each generation.
- *Number of generations*: The number of iterations the algorithm will go through.
- *Selection pressure*: Higher values will assign more weight to structures with a higher fitness when applying genetic operators.
- *Number 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

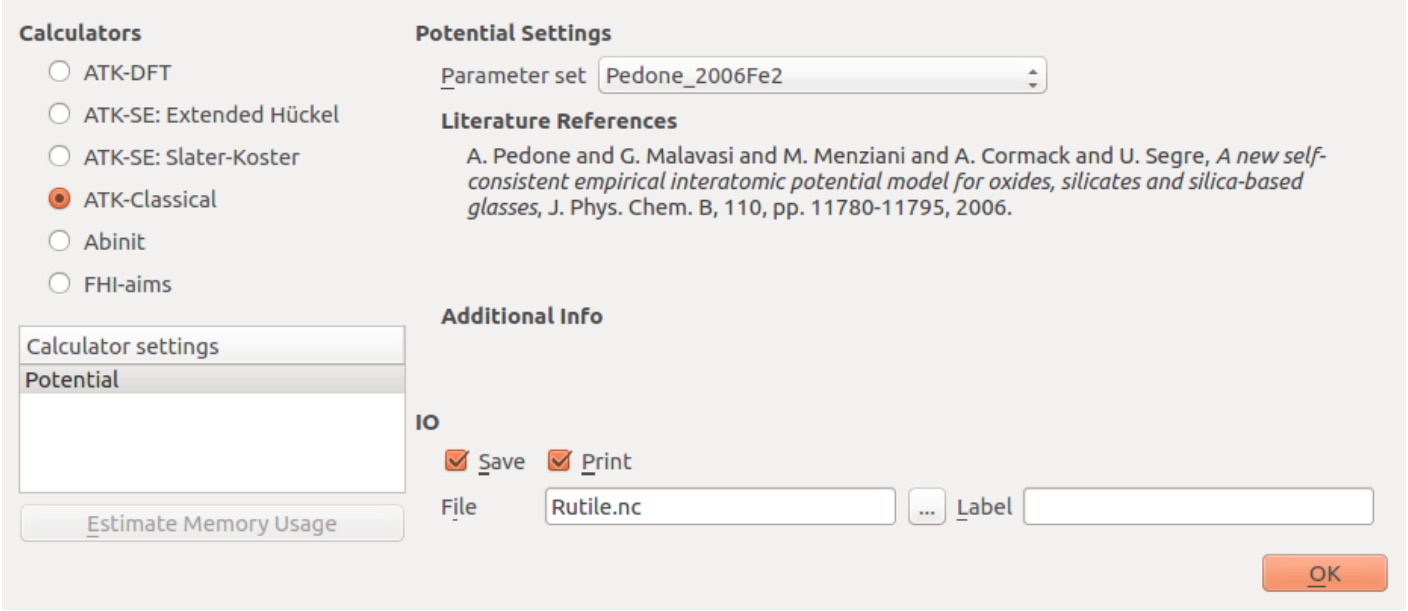
⊙Genetic Operators:

- *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*.



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



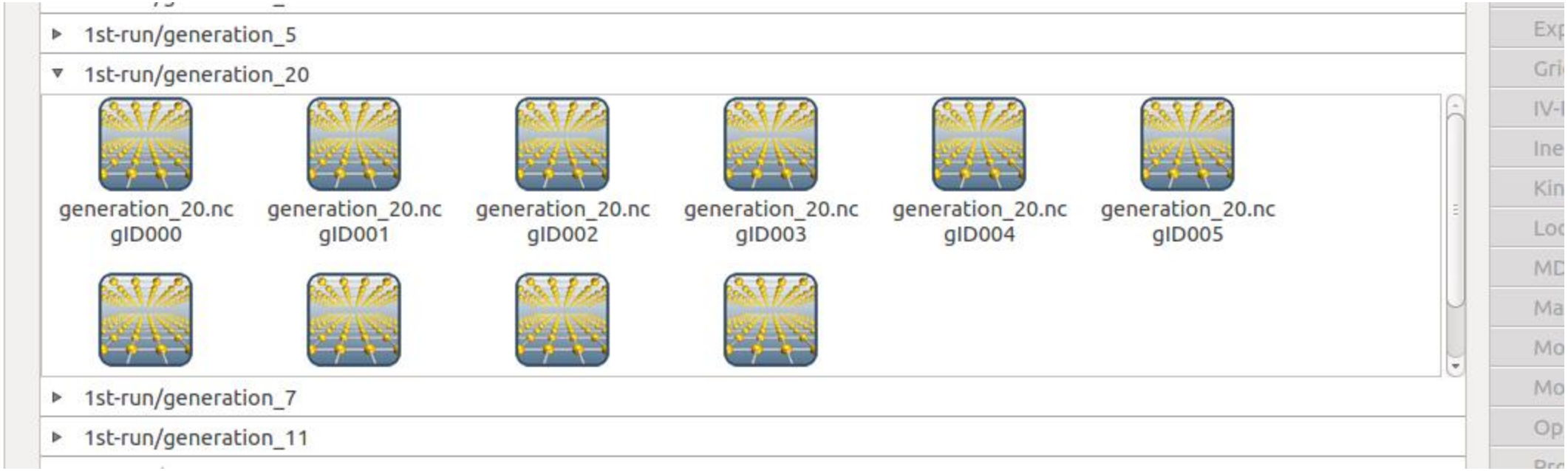
Results – main log-file

- *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.

```
+-------------------------------------------------------------------------------+
| Niching                                                                       |
+-------------------------------------------------------------------------------+
| Killing individual  0                                                         |
| Killing individual  1                                                         |
| Killing individual  4                                                         |
| Killing individual  6                                                         |
+-------------------------------------------------------------------------------+
| Population for Final Niched Generation                                        |
+-------------------------------------------------------------------------------+
| Individual   0: Fitness:   94.238940                                          |
|                 Symmetry:  P4_2/mnm       Volume:     63.5550                 |
|                 Max Force: 0.0056         Max Stress Error: 0.0929            |
|                 History: IPPPPPPPPPPPPPPPPPPP                                 |
| Individual   1: Fitness:   93.978255                                          |
|                 Symmetry:  I4_1/amd       Volume:     70.0359                 |
|                 Max Force: 0.0025         Max Stress Error: 0.0380            |
|                 History: IPPPPPPPPPPPPPPPPPPP                                 |
| Individual   2: Fitness:   93.796305                                          |
|                 Symmetry:  Fd-3m          Volume:     139.6049                |
|                 Max Force: 0.0099         Max Stress Error: 0.0357            |
|                 History: IXPPPPPPPPPPPPPPPPPP                                 |
| Individual   3: Fitness:   93.625090                                          |
|                 Symmetry:  Cmcm           Volume:     87.9469                 |
|                 Max Force: 0.0074         Max Stress Error: 0.0533            |
|                 History: IPPPPPPPPPPPPPPPPPPP                                 |
| Individual   4: Fitness:   93.388660                                          |
|                 Symmetry:  Imcm           Volume:     100.2970                |
|                 Max Force: 0.0092         Max Stress Error: 0.0912            |
|                 History: IPPPPPPPPPPPPPPPPPPH                                 |
| Individual   5: Fitness:   92.364891                                          |
|                 Symmetry:  Imm2           Volume:     86.5277                 |
|                 Max Force: 0.0042         Max Stress Error: 0.0761            |
|                 History: IPPPPPPPPPPPPPPPPPPH                                 |
+-------------------------------------------------------------------------------+
| Legend: I=Initial P=Promotion H=Heredity M=Mutation X=Permutation             |
|         fitness in units of eV                                                |
|         force   in units of eV/Angstrom                                       |
|         stress  in units of GPa                                               |
+-------------------------------------------------------------------------------+
```

Results

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



Thank You!

Quantum Wise