

Running USPEX with ATK (tutorial by X. Dong)

Introduction

The USPEX code (Universal Structure Prediction: Evolutionary Xtallography) can be used to predict stable crystal structures at given conditions, knowing only the chemical composition. USPEX can also be used for finding low-energy metastable phases, as well as stable structures of nanoparticles, surface reconstructions, molecular packings in organic crystals, and for searching for materials with desired physical (mechanical, electronic) properties. The USPEX code is based on an efficient evolutionary algorithm developed by A.R. Oganov's group, but also has options for using alternative methods (random sampling, metadynamics, corrected PSO algorithms, nudged elastic band, et al).

Now USPEX is also interfaced with ATK. Note that USPEX only calls the ATK standalone mode, not visual program VNL. The following text shows how to use USPEX+ATK to predict the structure of elemental silicon with 8 atoms per cell using DFTB calculations available in ATK. DFTB is a very attractive option as it combines very high speed with often acceptable accuracy and can be used for large systems.

Preparation

As in any USPEX calculation, **INPUT.txt** and **Specific** folder should be prepared in the same folder where you find USPEX.m. Also for parallel edition, **Submission** folder should be adjusted for your specific job-scheduling system. For a detailed description, please register on the USPEX website (<http://uspex.stonybrook.edu/uspexdownloads.php?id=0&code=1000>) and download USPEX and its comprehensive manual.

The following example is for a serial calculation. Note that “serial” here means that structures are relaxed one at a time – but for this relaxation you can use many CPUs using MPI-parallelization of ATK.

We recommend that when you prepare your calculation, you start with one of the already prepared test cases and modify it. For example, there is Test20_ATK, which uses USPEX in conjunction with ATK.

INPUT.txt:

abinitioCode should be set as 10 (this sets ATK as the code of your choice). And the number of 10 equals to how many steps do you want for one structure.

When setting ATK execution command, the input file name should be ATK.in and output file name should be ATK.out. For serial edition the command will be set as commandExecutable in INPUT.txt; for parallel edition the command will be set in Submission/submitJob_local.m.

All other settings will be the same as in usual USPEX calculations. Some important parameters that are specific for each system are: numSpecices, atomType, Latticevalues, et al.

Specific folder:

The fold Specific contains the ATK input files, ATK_input_1...n, n equals the number of stages of relaxation that you set in INPUT.txt. All files should be the normal ATK files for optimizing geometry with all parameters except atomic coordinates, cell parameters (these will be written by USPEX at the head of the file). **At the end of these input files, bulk_configuration and TotalEnergy should be output for USPEX to read.**

An example of ATK_input_5 file is as follow:

```
#####  
# setup slater-koster calculator with dftb parameters  
basis_set = DFTBDirectory("/gpfsHOME/home/dx2/QuantumWise/atk-12.8.2/atkpython/share/  
tightbinding/cp2k/nonscc/") #basis set
```

```
pair_potentials = DFTBDirectory("/gpfsHOME/home/dx2/QuantumWise/atk-12.8.2/atkpython/  
share/tightbinding/cp2k/nonscc/") #pair potentials
```

```
numerical_accuracy_parameters = NumericalAccuracyParameters(  
    k_point_sampling=(8, 8, 1),  
) #if k_point_sampling is found, whatever is defined by it, it will be superseded by the k-  
points grid created by USPEX using settings specified in INPUT.txt
```

```
calculator = SlaterKosterCalculator(  
    basis_set=basis_set,  
    pair_potentials=pair_potentials,
```

```

numerical_accuracy_parameters=numerical_accuracy_parameters,
) #calculator
bulk_configuration.setCalculator(calculator) #The calculator is
bulk_configuration = OptimizeGeometry(
    bulk_configuration,
    maximum_forces=0.001*eV/Ang,
    max_stress=0.005*eV/Ang**3,
    max_steps=50,
    disable_stress=False,
) # Optimize geometry is the most important procedure, max_stress and max_steps are used
for cell optimize of crystal, when disable_stress=False.

```

```

# -----
# energy and structure output
# -----
total_energy = TotalEnergy(bulk_configuration)
nlprint(total_energy)
nlprint(bulk_configuration)
#stress=Stress(bulk_configuration)
#nlprint(stress)
#####

```

We recommend to do a coarse calculation as the first stage of relaxation and gradually increase precision of relaxation, step by step. When crystal calculation is performed, a fixed-cell calculation (`disable_stress=True`) is also suggested in `ATK_input_1`. Each higher-level structure relaxation starts from the results of a lower-level relaxation. The settings of each `ATK_input` can be found in our tutorial `T20_ATK`.

Because USPEX often starts relaxation very far from local minimum, you should ensure that your calculator, basic sets and potentials will not give too bad long-range or short-range interactions. Very bad long-range or short-range interactions will lead the ATK calculation to endless loop or give some unreasonable energy value.

Calculation

You can use matlab (`matlab < USPEX.m > log`) or octave (`octave < USPEX.m > log`) to call USPEX.

If your setting is correct, folder named **results*** (result folder) and **CalcFold*** (calculation folder) will be created, and then ATK calculation will start. The details about the files in result folder can also be found in USPEX manual.

If USPEX or ATK doesn't work or you have any other problem, please check whether the **ATK.in** file in **CalcFold1** is right and executable, and if the problem persists, then contact us.

Results

In our example the ground-state structure was found in the 8th generation.

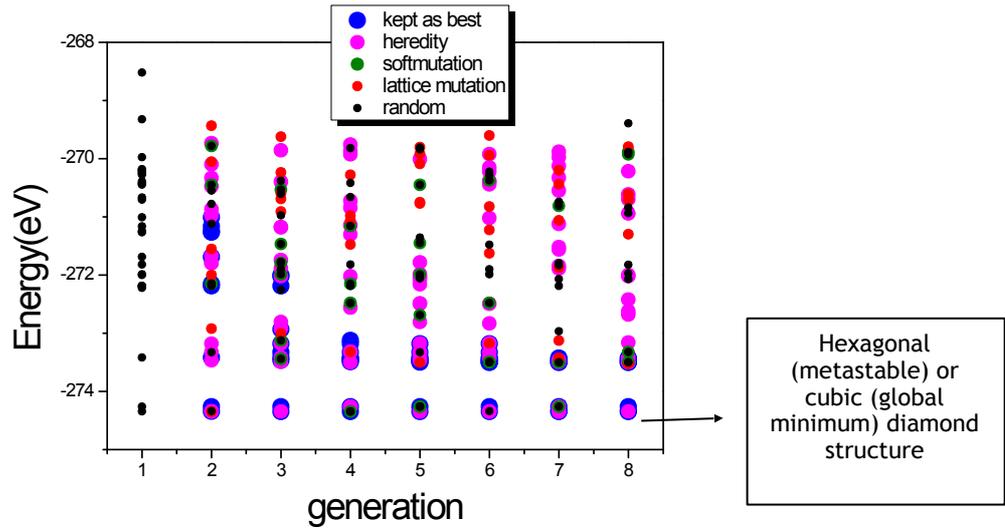


Fig. 1: Evolution of a population of Si structures.

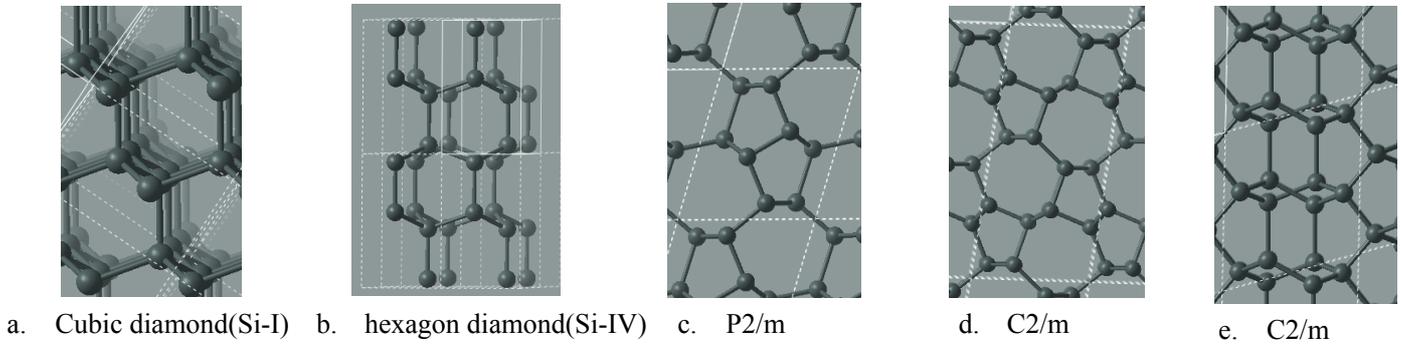


Fig. 2 the first five structures in `result1/goodStructures_POSCARS`.

Fig. 1 shows that our algorithm is extremely efficient. Fig. 2 shows the five different structures with lowest energy. By the way, if you are predicting metastable structures, we recommend calculating more generations (increase `stopCrit` in `INPUT.txt`), even though the best structure is found quickly, it may be worthwhile continuing the calculation to wait for more metastable structures to be found.