MTB TMD Generator

This PYTHON application generates a POSCAR file for a unit cell of 4|4P mirror twin boundary (MTB) triangular structures for a given transition metal dichalcogenide (TMD).

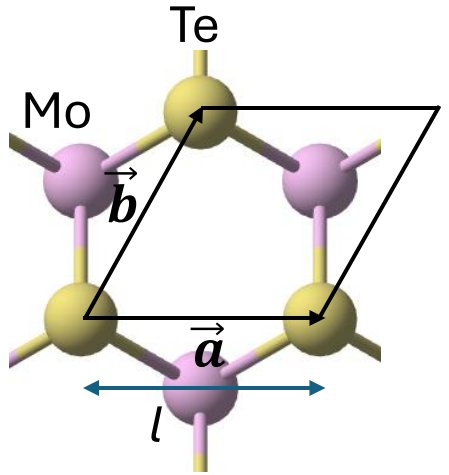
Daniil Kruklinskii

The program uses a config.txt file to read all the necessary input data

Each line contains the following data:

1. Chemical symbol for the transition metal.
2. Chemical symbol for the chalcogen.
3. Lattice parameter in angstrom (distance between neighbouring atoms of the same species).
4. Vertical distance between the two chalcogens in a unit cell in angstroms.
5. Vertical vacuum separation between TMD layers in angstroms.
6. Size of MTB triangle edge in units of lattice parameter (integer).
7. Superlattice vector 1 (three integers separated by spaces).
8. Superlattice vector 2 (three integers separated by spaces).

The program uses a config.txt file to read all the necessary input data

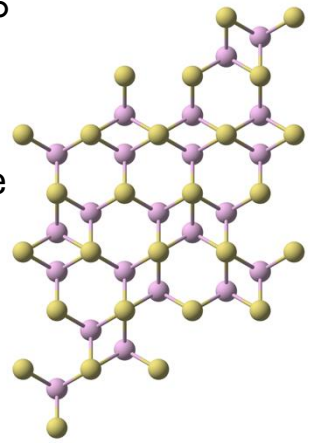
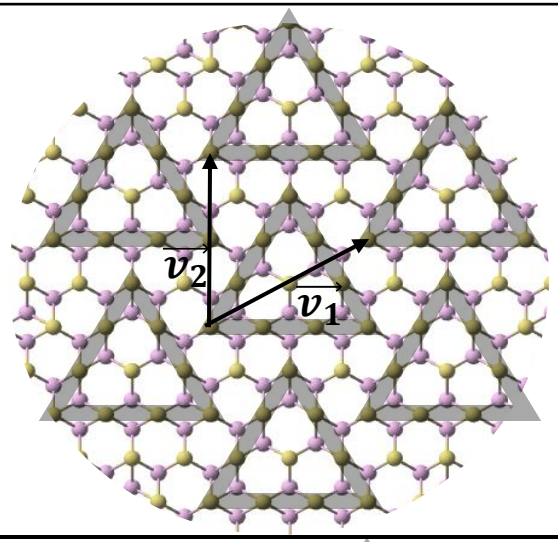
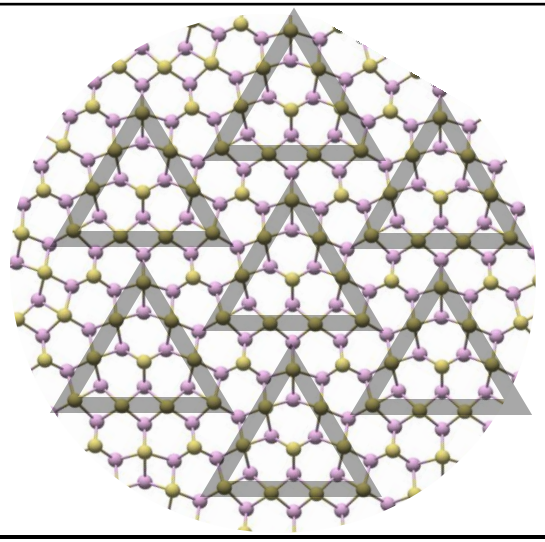
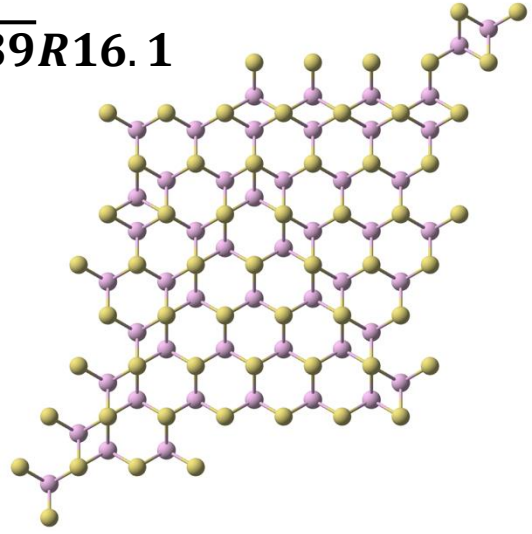
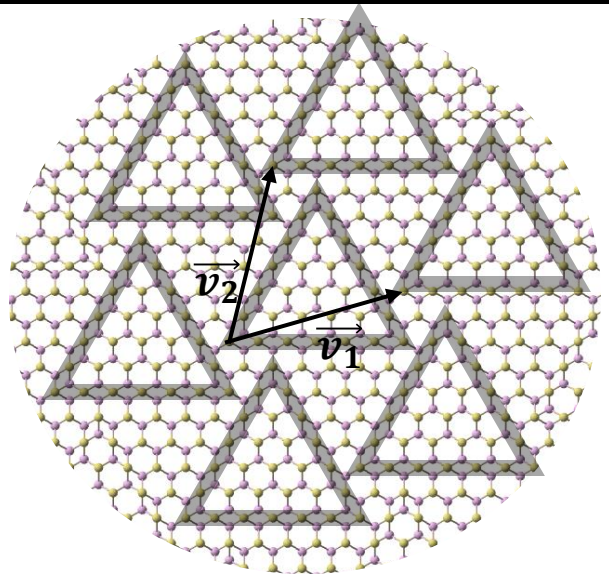
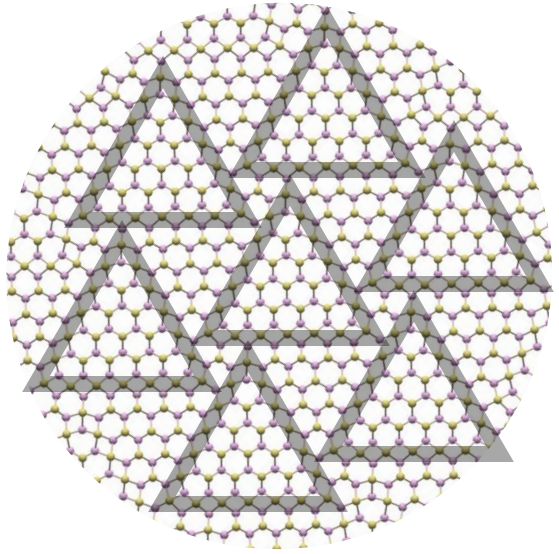


config.txt format remarks:

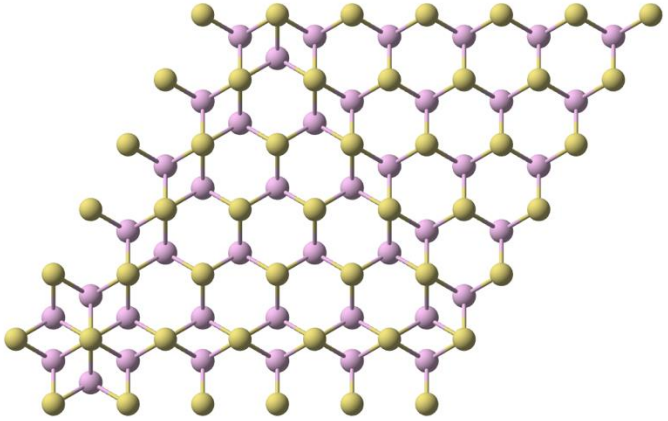
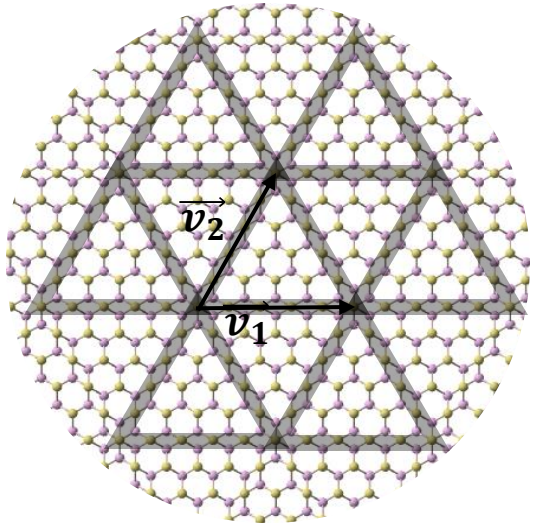
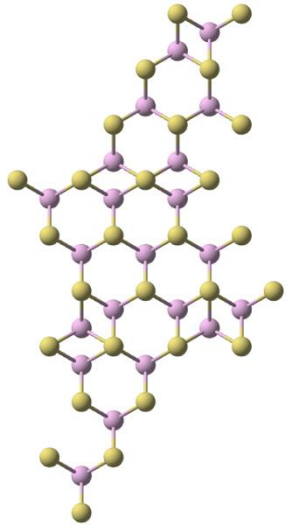
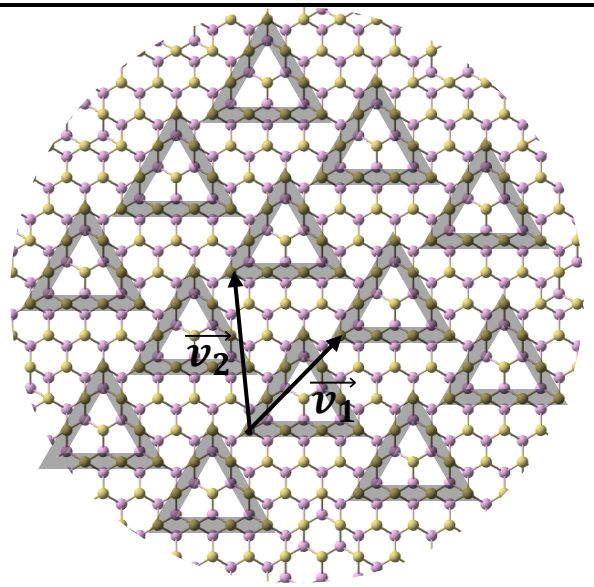
- The config file must be in the same working directory as the script itself.
- The name of the config file must be strictly "config.txt".
- The config file must contain all eight data entries on separate lines.
- Avoid anything that does not adhere to the config format.
- Avoid unnecessary spaces.
- The superlattice vectors in (7) and (8) define the lattice vectors of the new system and are to be written as three numbers separated by spaces, e.g. "1 2 0".
- Superlattice vectors are defined as fractional coordinates of the original TMD lattice vectors $\boldsymbol{a} = (l, 0, 0)$, $\boldsymbol{b} = (l/2,\ l\sqrt{3}/2, 0)$ and $\mathbf{c} = (0, 0, vacuum)$ where l is a lattice parameter in (3).

All this information is also provided in README.md file

Examples

Config.txt	Primitive unit cell (produces by the script)	Supercell (for visualization)	Supercell of the optimized structure
Mo Te 3.52 3.40 20 3 2 2 0 $\overrightarrow{v_1}$ -2 4 0 $\overrightarrow{v_2}$ Triangle edge length	$2\sqrt{3}R30°$ 		
Mo Te 3.52 3.40 20 6 5 2 0 -2 7 0	$\sqrt{39}R16.1$ 		

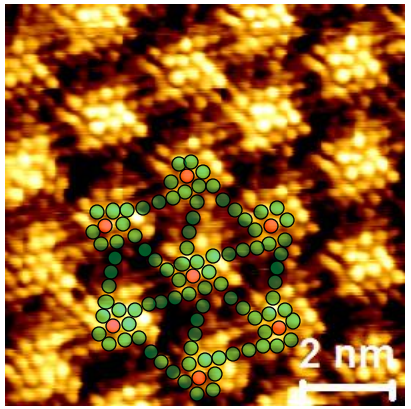
Examples

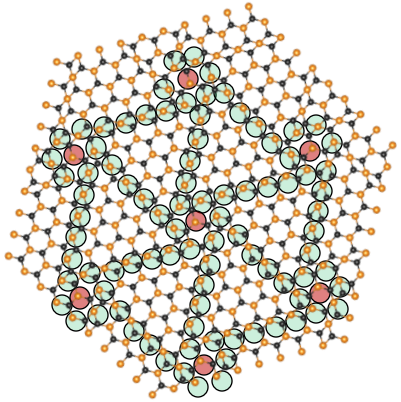
Config.txt	Primitive unit cell (produces by the script)	Supercell (for visualization)
Mo Te 3.52 3.40 20 5 5 0 0 $\overrightarrow{v_1}$ 0 5 0 $\overrightarrow{v_2}$		
Mo Te 3.52 3.40 20 3 1 3 0 -3 5 0		

Triangle edge length

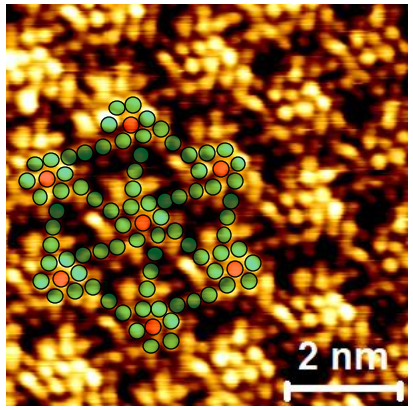
STM

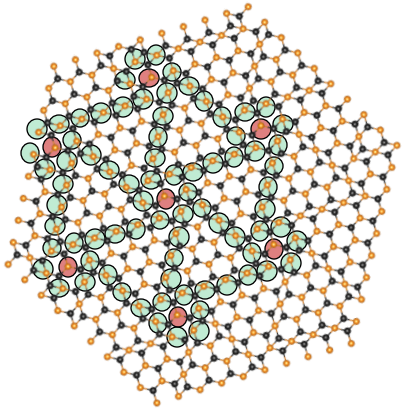
$\sqrt{39}R16.1$



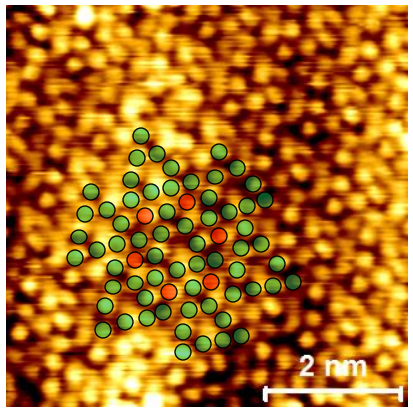


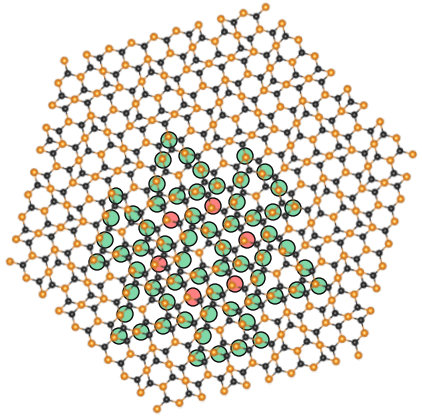
$2\sqrt{7}R19.1°$





$2\sqrt{3}R30°$





STM Simulation