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This directory contains some files for the Stillinger-Weber (SW) potential, especially the parameterization of the SW potential for 2D nano-materials.

(*). 2018 Misfit Strain-Induced Buckling for Transition-Metal Dichalcogenide Lateral Heterostructures: A Molecular Dynamics Study(amss).pdf

SW potential for MX₂ compounds, published version.

(*). sw_mx2.zip:

The compressed file, containing source files for the above paper on SW for MX₂ compounds, including an example to run MD simulations using LAMMPS.

(*). 2017 Handbook of Stillinger-Weber Potential Parameters for Two-Dimensional Atomic Crystals(intech)-1.pdf

2017 Handbook of Stillinger-Weber Potential Parameters for Two-Dimensional Atomic Crystals(intech)-2.pdf

SW potential for 156 2D nano-materials, published version in IntechOpen, first and second parts.

(*). supplement.zip:

The compressed file, containing all supplemental materials for the above paper on SW for 156 2D nano-materials, including a fortran code to generate crystals' structures, files for molecular dynamics simulations using LAMMPS, files for phonon calculations with the SW potential using GULP, and files for phonon calculations with the valence force field model using GULP.