

Microkinetic Modeling

Installation

NOTE: The "micro-kinetics module" (mkm) is now deprecated. The new version has been re-named to [CatMAP](#). Old versions of mkm will remain on svn indefinitely for those who may wish to re-run older scripts.

The kinetics modeling package is currently in alpha-testing and is available only via SVN. In order to access the package you will need the following dependencies:

svn (for installing and updating)
python (version 2.5 or greater)
python modules:

- numpy
- scipy
- mpmath
- ase
- gmpy (optional - gives 2-3x speedup for multiple precision calculations)

You can then install the module via svn with the following command in the terminal:

```
svn co svn://suncatls1.slac.stanford.edu/kinetics/trunk <packagename>
```

where <packagename> is the name of the local directory where the module will be stored. After installing you can get the most current version of the package by going into the <packagename> directory and typing:

```
svn update
```

As the package is currently under development, some issues and bugs are to be expected. If you are interested in working on the module as a developer please send a message to the developers list mkm-developers@stanford.edu to obtain read/write access.

Contents

The trunk contains 4 different python modules. Two are current:

- simplekinetics - A collection of less automated but easier to read micro-kinetic modeling scripts written by Simon Brodersen
- mkm - The most current version of the "micro-kinetics module"

and 2 are provided for backwards compatibility and are no longer maintained:

- mkm_0 - A version of the "micro-kinetics module" which is compatible with inputs from before July 25, 2013 (note that any imports of mkm will need to be changed to mkm_0 for the old scripts to work)
- kinetics - A version of the "micro-kinetics module" which is compatible with inputs from before February 10, 2013 (note that in these scripts the mkm module is instead called "kinetics")

Both of these deprecated packages will be removed in releases greater than 0.2.X.

License and Citation

The code is available under the GNU General Public License agreement (version 3). You can cite this package with the following information:

- Authors: Andrew J. Medford, Simon Brodersen, et. al.
- Title: Micro-kinetics Module
- Year: 2013-
- URL: suncat.slac.stanford.edu/software/
- Version: 0.1.XX (where XX corresponds to the SVN revision used)

Documentation

A general overview can be found on the [Overview](#) page, and some [Tutorials](#) are also available. Please send any questions to mkm-developers@lists.stanford.edu, but check the [archives](#) first to make sure your question hasn't already been answered.