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1.1 Introduction

scikit-nano is a python toolkit for nano-science. Currently, its primary use is for generating nano-structure data for the following nano-materials:

• Graphene, both single layer graphene and N-layer graphene.
• Single-walled nanotubes (SWNTs), both single SWNTs and SWNT bundles.
• Multi-walled nanotubes (MWNTs), both single MWNTs and MWNT bundles.

It supports saving structure data in the following formats:

• xyz
• LAMMPS data

I’ve adopted the scikit- naming convention for this project in hopes of contributing it to the collection of SciKit libraries in the near future.

1.2 Installation

1.2.1 Required Dependencies

• Python 2.7+
• VMD (for visualizing structure data)
• Tachyon (for rendering high quality images)

1.2.2 Installing scikit-nano

You can install the latest stable release from the Python Package Index using pip:

> pip install sknano

Alternatively you can download a source code tarball from http://pypi.python.org/pypi/sknano or clone the source code from the github repository using git:

> git clone https://github.com/androomerrill/scikit-nano.git
cd into the source code directory and run:

> python setup.py install

These commands will probably fail if you don’t have *admin privileges*. In that case, try installing to the user base directory. Using **pip**:

> pip install --user sknano

Or from source:

> python setup.py install --user
2.1 Generating nanostructures (*sknano.nanogen*)

This tutorial describes the modules available in the *sknano.nanogen* sub-package.

2.1.1 Structure generators

The *nanogen* module provides the following classes for structure generation:

- GrapheneGenerator
- BiLayerGrapheneGenerator
- NanotubeGenerator
- TubeGen

2.2 scikit-nano scripts

The tutorials below describe the scripts available in the *scripts* package.

2.2.1 scikit-nano script tutorial: *sknano.scripts.nanogen*

2.3 Examples

Write script to walk the module tree, parse example content from docstrings, autogenerate literalincludes directive, and reproduce the content here.
Contribution to scikit-nano

As any non-cave-dwelling developer knows, working on a project alone sucks. Collaboration inspires new ideas, leads to better code, and increases the longevity of a project. I welcome any and all constructive feedback and anyone interested in contributing code, please email me or consider forking the project on github and submitting your contribution with a pull request. Thanks!
Release Notes
5.1 website template

As the saying goes, “imitation is the sincerest form of flattery,” and all credit for this website’s template goes to the authors of the scipy documentation template.
6.1 pykit projects

- pykit-sci docs
- pykit-shared docs
- genindex
- modindex
- search