
addisnano Documentation

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CHAPTER 1

Benchmark Datasets

There are several dataset benchmarking in addisnano software to k provides convenient interfaces to popular benchmark datasets

- QM9
- QM8
- QM7b
- QM7
- MD7

Installation

Addisnano is a Deep Tensor Learning Neural Network to the prediction of potential energy surfaces and other quantum-chemical properties of molecules and materials in atomistic system. It contains basic building blocks of atomistic neural networks, manages their training and provides simple access to common benchmark datasets. This allows for an easy implementation and evaluation of new models.

We can install the application with pip as:

1. `$ pip install addisnano`
2. `$ conda install -c conda-forge addisnano`

CHAPTER 3

Indices and tables

- genindex
- modindex
- search