WP1: material science The big picture: NoMaD Laboratory

http://nomad-repository.eu



/elcome to the NoMaD Repository



ne years ago.

> NoMaD Repository enables the confirmatory analysis of materials data, their reuse, and repurposing.

oad of data is possible without any barrier. Results are accepted in their raw format as produced by the lerlying code. The only condition is that the list of authors is provided, and code and code version can be ieved from the uploaded files. These data can be restricted to the owner or made available to other people lected by the owner). They can be updated and downloaded at any time.

ad more details concerning the upload. Please, **register** or **login** to ticipate.

present, the repository contains *ab initio* electronic-structure data from isity-functional theory and methods beyond. At a later stage, it will be ended by force-field studies and by experimental data. We also give an look on the *NoMaD Laboratory* that will be dedicated to a *Materials cyclopaedia*, as the basis for complex queries and the development of lous data-analytics tools.

ALTS AND ALTERIALS OF THE POPPE

The *NoMaD* (Novel Materials Discovery) *Repository* was established to host, organize, and share materials data.

NoMaD copes with the increasing demand and requirement of storing scientific data and making them available for longer periods. Rules of good scientific practice set by many funding agencies, worldwide, require keeping scientific data for 10 years. **NoMaD** offers this for free. **NoMaD** also facilitates research groups to share and exchange their results, inside a single group or between two or more, and to recall what was actually done Discovery (NoMaD) Repository, materials data are stored raw, as they are output by atomistic-simulation codes.

In the Novel Materials

Open positions

News

entries.

Check for related conf and workshops.

Currently, the NoMaD

Repository contains 2

NoMaD registered at

We are making NoMal powerful and apologize possible instability dur time.

The NoMaD Repositor about joining eudat.

Financial Support

Its purpose is to enable

- confirmatory analysis
- reuse
- repurposing
 of materials science
 data.

The big picture: NoMaD Laboratory

E.g., NoMaD Repository, other repositories

Output:

data in a representation independent of the specific (atomistic-simulation) code that produces them

Discovery of new descriptors

Encyclopaedia: SQL db



First step of NoMaD Lab: Conversion Layer (Normalized Data)

- Meta data to describe and uniquely identify stored data
- Sha224 based identifier for meta data to allow extensibility while avoiding clashes
- https://www.hdfgroup.org/HDF5/ To store values (efficiently store multidimensional arrays)
- Hope to use experimental Single Writer Multiple Readers feature in the future
- Active data can only get new data, not remove old

NoMaD Laboratory Base Layer

- Reactive application using http://akka.io/
- http://spray.io/ To give an http interface to the service
- Flink used for stream processing and querying
- Extensive use of sha224 based identifiers:
- File/archive identifiers
- Calculation identifiers
- Meta data identifiers
- Formatting independent json/HDF5 identifiers
- Server address independent URIs to refer to all data

NoMaD Laboratory Base Layer

