

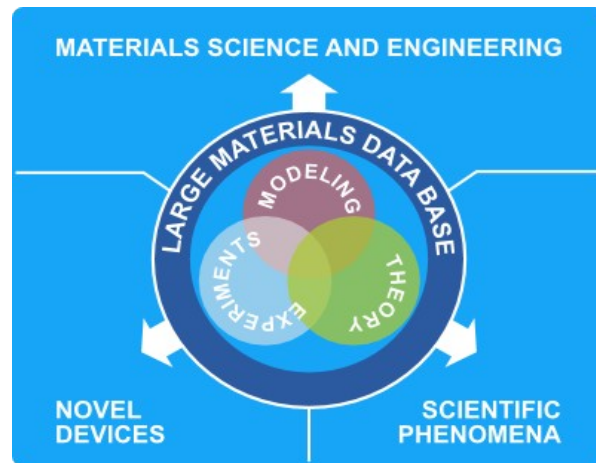
# Nomad, the Novel Materials Discovery laboratory

Rosendo Valero<sup>1</sup>, Ask Hjorth Larsen,<sup>2</sup> Stefan Bromley,<sup>3</sup> Francesc Illas<sup>4</sup>

<sup>1,2</sup> Departament de Química Física, Universitat de Barcelona, *Barcelona, 08028, Spain*

E-mail: rosendo.valero@ub.edu

The Nomad laboratory is a European Center of Excellence (CoE) [1] funded by the European Union under the Horizon2020 program. The project involves eight computational materials science groups and four high-performance computer centers. The final purpose of the initiative is to facilitate the discovery of new scientific phenomena and novel devices, and the advancement of materials science and engineering. The Nomad CoE starts from the *Nomad Repository* [2] which contains at present more than 3 million input and output files generated by high-quality programs all over the world. As the data are very inhomogeneous, a parsing and conversion layer is first developed, which constructs a code-independent database for the purpose of data analytics. Then, a *Materials Encyclopedia* is envisaged, which will be formed by the large materials data pool and fast search engines to retrieve those materials with one or more required features. The core of the project is the *Big-Data Analytics* tool. This tool will extract hidden structures and correlations from the data, thus discovering trends and anomalies and even novel materials. The tools employed for this endeavor are data mining and statistical or machine learning. A centralized visualization service will enable users to interactively perform data visualization on their computers without having to rely on their own hardware and software installations. Finally, we aim at stimulating widespread interest on the Nomad CoE through industrial and researcher networking, and public awareness (with a project website, a project documentary and press releases, among other initiatives).



**Figure 1.** Scheme of the Nomad laboratory.

## Bibliography

[1] <https://nomad-coe.eu/>

[2] <http://nomad-repository.eu/cms/>