



## NOMAD Centre of Excellence launches the NOMAD Encyclopedia

The [NOMAD Laboratory Centre of Excellence](#) (CoE) has officially launched a freely accessible knowledge base on the computed properties of materials, the [NOMAD Encyclopedia](#), which acts as a user-friendly interface for accessing the project's extensive data collection. It is based on the [NOMAD Repository](#), a platform for hosting, organising, and sharing calculational data originating from a variety of methods and programs. Comprising more than 3.4 million calculations, it is the largest database of computed materials data worldwide.

The NOMAD CoE, of which Barcelona Supercomputing Center (BSC) is a consortium member, also converts this data into a code-independent and uniform format, stored in the [NOMAD Archive](#). This database serves as the base for tools for advanced visualisation and big data analytics, while the Encyclopedia provides materials-oriented access points to the data.

This [video](#) gives an overview of the NOMAD CoE.

### **A graphical user interface for everybody**

Build for scientists as well as non-experts, the Encyclopedia graphical user interface (GUI) makes this massive materials knowledge searchable and visible. To achieve this, the interface has been developed with the input of BSC's user experience and design experts. The result is an intuitive web application that allows users to search for chemical elements, a material's chemical formula, or specific properties. For every material, a general characterisation is provided as well as further details specific to that material. Additional features like downloadable virtual reality files of atomic structures can help teachers make science lectures more engaging, as well as providing a resource for experts examining complex materials for new sources of electric energy.

**Georg Huhs**, researcher at the Computer Applications in Science & Engineering (CASE) department at BSC, has had a leading role in the creation of the NOMAD Encyclopedia. According to Georg: "The success of NOMAD in collecting and opening up such a large amount of materials data is impressive. To extract the value hidden in them, these data have to be made visible and explorable in a user-friendly way. This is what the Encyclopedia does. What we have built until now is only the beginning. With time, we will expand the characterisation of the materials, add more and more different types of materials, and even provide interactive tools to facilitate complex analysis tasks. One of the advantages of this project is that such additions may be developed just for a special interest, for example in collaboration with an industrial client, but automatically become available for this huge dataset and for all users."

### **The API - also designed for robots**

All the data of the Encyclopedia are also accessible via an open, web-based Application Programming Interface (API). This gives every user more options for using the Encyclopedia data. For example, one can download a dataset to plot data in a different environment, or even use



them as input data for further calculations. Customers can even build their own applications, accessing the Encyclopedia API as a data source. This is extremely useful for applications in science and industry, such as researching new photovoltaic panels or engineering materials under extreme conditions.

The NOMAD CoE will keep growing its data content and contributing to the computational materials science community. Every six months, meetings with the scientific advisory committee and industry advisory committee are organised in order to discuss users' needs and the next steps of the project. The last scientific [meeting](#) was hosted by BSC and took place on 3-5 October 2016.

### **About the NOMAD CoE**

The NOMAD CoE is a European-funded project, which includes Barcelona Supercomputing Center, Max Planck Society, King's College London, Humboldt University of Berlin, University of Cambridge, University of Barcelona, Aalto University, Technical University of Denmark, Leibniz-Rechenzentrum, CSC – IT Center for Science, and Pintail Ltd. The project started in November 2015 and is planned to finish on October 2018, funded by the European Union's Horizon 2020 research and innovation programme under grant agreement no. 676580 with a budget of €4.9 million.

[www.nomad-coe.eu/](http://www.nomad-coe.eu/) | [www.twitter.com/NoMaDCoE](https://www.twitter.com/NoMaDCoE) | [www.facebook.com/nomadCoE](https://www.facebook.com/nomadCoE) | [www.linkedin.com/company/nomadlaboratory](https://www.linkedin.com/company/nomadlaboratory) | <https://www.researchgate.net/project/The-NOMAD-Laboratory-a-European-Centre-of-Excellence>

### **About the NOMAD Repository**

To find out more about the unique Repository of computational materials science data, watch the following [video](#).