Project Partners

Eight complementary research groups of the highest scientific standing in computational materials science along with four high-performance computer centers form the synergetic core of this European Centre of Excellence.

Fritz Haber Institute of the Max Planck Society

Max Planck Computing and Data Facility

Max Planck Institute for the Structure of Dynamics of Matter

King's College London

Humboldt University

University of Cambridge

University of Barcelona

Aaalto University

Technical University of Denmark

Leibniz-Rechenzentrum

CSC – IT Center for Science

Barcelona Supercomputing Centre

Pintail Ltd

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Project Facts

Duration: 3 years
Start Date: 01 Nov 2015

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http://nomad-coe.eu/

NOVEL MATERIALS DISCOVERY

The Novel Materials Discovery Laboratory

NOMAD

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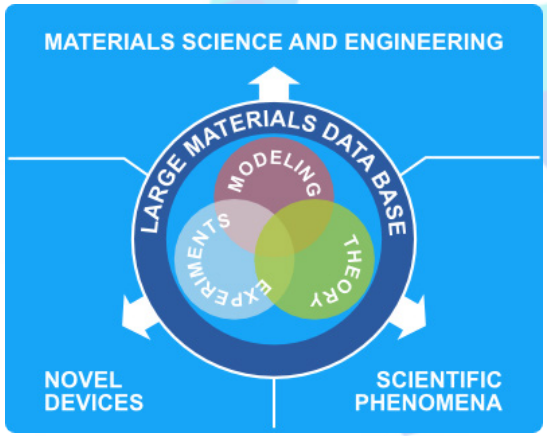
What is computational materials science?

Computational materials science is the exploration of how materials behave, based on what we know about atoms and molecules and using quantum mechanics. Understanding and predicting how materials behave is important so that we can choose the best materials to make new or improved commercial products, such as more efficient solar panels, longer-lasting artificial joints or lighter, more durable smartphones. Using powerful computers, computational materials scientists can predict which materials will work best for different applications and even consider materials that do not yet exist.

In computational materials science, complex methods and codes are used to generate large amounts of data. There is already a lot of data available for many materials, but they are stored in different places all over our planet and in different formats, making it hard to integrate and use. To make it easier for researchers in industry and universities to use this data, the NOMAD Centre of Excellence (CoE) will gather and integrate existing computational materials science information into a single, virtual centre - the NOMAD Laboratory.



NOMAD Laboratory

NOMAD is part of the integrated high performance computing (HPC) programme of Horizon 2020, building on HPC capabilities from the Fritz-Haber-Institute of the Max Planck Society, Max Planck Institute for the Structure of Dynamics of Matter, Max Planck Computing and Data Facility, Humboldt University and Leibniz-Rechenzentrum Garching. Using this existing HPC infrastructure, the NOMAD Laboratory will provide users with a **Materials Encyclopedia, Big-Data Analytics Toolkit** and **Visualisation Tools**.

Materials Encyclopedia

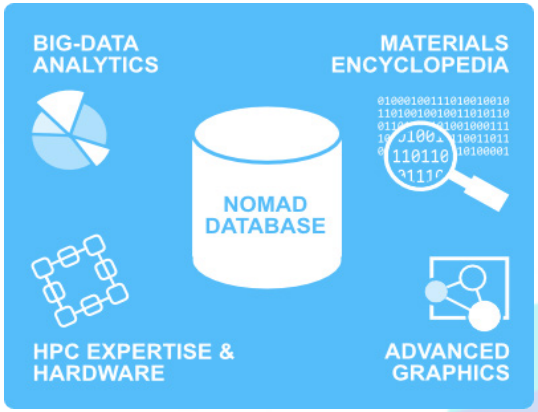
The Materials Encyclopedia will provide comprehensive information on materials and their computed properties. We will first develop an efficient strategy for managing and accessing the large quantities of data already available in repositories across Europe. We will then develop an approach to translate the data to a common, code-independent format. Data will then be converted, compressed and stored in a scalable database that will be the backbone of the Encyclopedia. A user-friendly search engine will allow users to complete complex queries of the database, which they can access using the Visualisation and Big-Data Analytics tools that we develop during the project. Using these tools, users will be able to search for and identify materials with particular properties, for particular applications.

Big-Data Analytics

The NOMAD database will contain large amounts of data ('big data') that will allow researchers and other users to identify and understand correlations, discover hidden trends and identify materials that may have unique and useful characteristics. The key challenge is to develop tools that can effectively harness the potential of our large, code-independent database. The tools will be ready to use through the Materials Encyclopedia, but will also be easy to embed in more complex analysis codes.

Advanced Graphics

NOMAD will develop **software for remote visualisation** of our multi-dimensional data. Users will be able to perform comprehensive data visualisation tasks on their own computers, without the need for specialised software or hardware. Visualisations will include chemical structures, spatial data and abstract data. A **virtual reality environment** will also be developed to allow interactive data exploration, training and dissemination.



Outreach

NOMAD includes an array of industrial networking and outreach activities to reach users who can benefit most from the NOMAD Laboratory, including manufacturing-driven companies and software companies. We aim to:

- maximise the industrial relevance of our work,
- improve active uptake of our results by key industries,
- generate and promote support resources that target those with an interest but not experience in computational materials science, and
- promote the competitiveness of EU-based industry.

NOMAD will also include outreach for the general public and mass media, policymakers, government agencies and other materials science and 'big data' researchers.