NOVEL MATERIALS DISCOVERY

# The Novel Materials Discovery Laboratory – NOMAD

## What is computational materials science?

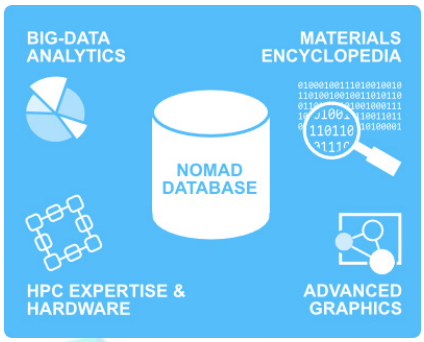
Computational materials science is the exploration of how materials behave, based on what we know about atoms and molecules and using quantum mechanice. Understanding and predicting how materials behave is important so that we can choose the best materials to make new or improved commercial products, 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.

## What will be available in the NOMAD Laboratory?

Using existing European high performance computing (HPC) infrastructure, the NOMAD Laboratory will deliver:

- A **Materials Encyclopedia** that will provide comprehensive information on materials and their computed properties, based on a scalable database compiled from data from existing repositories across Europe. The Encyclopedia will allow us to efficiently manage and access large amounts of data ('big data').
- A **Big-Data Analytics Toolkit** with tools to allow academic and industrial users to use our large database to identify and understand correlations, discover hidden trends and identify materials that may have unique and useful characteristics.
- **Visualisation Tools** to allow users to visualise data on their own computers, without the need for specialised software or hardware. A virtual reality environment will also be developed to allow interactive data exploration, training and dissemination.




## How will NOMAD make a difference?

One of the key barriers to achieving the full impact of computational materials science is reaching the audiences that can benefit most, including a wide range of industries ranging from manufacturing-driven to software companies. The NOMAD CoE will involve our target end users through an array of industrial networking and outreach activities. In this way, we will maximise the industrial relevance of our planned developments, generate support resources that target those with an interest but not experience in computational materials science and promote the competitiveness of European industry. NOMAD will also include communication activities aimed at the general public and mass media, policymakers, government agencies and other materials science and 'big data' researchers.

http://nomad-coe.eu/ @NoMaDCoE www.facebook.com/nomadCoE

*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.*

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