

[BSC hosts the first Scientific Advisory Committee meeting of the NOMAD Centre of Excellence](#)



The [Novel Materials Discovery](#) (NOMAD) Laboratory, a Centre of Excellence (CoE), has held an internal meeting which gathered its principal investigators at the [Barcelona Supercomputing Center](#) (BSC) from 3 to 5 October. The agenda included the first meeting with NOMAD's **Scientific Advisory Committee** (SAC), formed of experts from the US, Japan and Europe.

BSC Computer Applications Department ([CASE](#)) researcher **Georg Huhs** explains that “it was a great opportunity to present the results of the first year's work and get feedback from well-known experts in the field. We also got an insight into related projects led by some of the SAC members”.

The NOMAD Centre of Excellence includes eight complementary research groups of the highest scientific standing in computational materials science along with four high-performance computing (HPC) centres which form the synergetic core of this CoE. BSC is one of these four core centres.

The NOMAD Laboratory takes its data from the NOMAD Repository, which is a [rapidly growing database](#) of computed materials data. Feel free to visit the “[Novel materials discovery repository](#)” video to find out more about the project.

BSC is working specifically on the [Materials Encyclopedia](#), which displays **computed materials properties**, based on a homogenized and normalized version of the NOMAD Repository data.

Whenever **new data** is available – whether concerning additional calculations, new materials or novel methodology - the NOMAD Encyclopedia will make it available to the outside world.

The information on individual materials will span from **structural and mechanical characteristics** to their **thermal behaviour** and from **basic electronic properties** to various kinds of **spectroscopy**. Likewise, complex queries will enable users **to find all possible materials in the database that possess the desired features**. To this end, the NOMAD team is developing a search engine together with a graphical user interface. After the first year of the project the whole data processing from the NOMAD Repository to a web-based graphical user interface of the NOMAD Encyclopedia has been accomplished and was presented at the meeting.

As BSC CASE Department Director, **José María Cela**, states: “an important aspect of the Centre of Excellence is to demonstrate its capacity to solve industrial problems. In this meeting several companies [which attended the event] has shown their interest in the activities of NOMAD and the use of this technology in their production process”.

Learning what industry wants and needs from NOMAD

Networking with industry is a key component of the project, so as to ensure that all of NOMAD's tools are relevant and accessible to industrial users. The Industry Advisory Committee includes representatives from SpringerMaterials, Haldor Topsøe, ONYX, QuantumWise, Dassault Systèmes BIOVIA, Fraunhofer, BP plc, Nokia Technologies, BASF SE and Max Planck Innovation. NOMAD has been conducting [one-to-one interviews](#) with decision-makers and technical R&D personnel to gain an even deeper understanding of industry needs and requirements to inform the development of the NOMAD Laboratory and the Sustainability Plan.

About NOMAD CoE

NOMAD CoE is led by Prof Matthias Scheffler of the Max Planck Society’s Fritz Haber Institute in Berlin. It includes seven other leading materials science centres, plus four supercomputing centres. The project is funded for an initial three years, for almost €5 million, under the EU’s Horizon 2020 programme.

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