

PRESS RELEASE

A new European **Centre of Excellence** will bring together physicists, chemists, materials, and computer scientists, and industry to develop a **Materials Encyclopaedia** and advanced tools for **Big-Data Analytics** to facilitate the discovery, creation and utilisation of **new materials**. The 'Novel Materials Discovery Laboratory' or **NOMAD**, will be 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 super-computing centres. The project is funded for an initial three years, for almost 5 million euro, under the EU's Horizon 2020 programme.

Materials science and engineering is the exploration of how materials behave and how they may be utilized in technological systems. New materials influence all aspects of our society, as they are important in the development of essentially every new commercial product, be it for better or novel solar panels, harder surfaces, lighter metals, and countless other applications. The number of different materials is very large - virtually infinite; so far we only know very few of those materials and the potential value of new materials is enormous.

NOMAD will develop a **Materials Encyclopaedia** that offers in-depth characterization of materials and their properties from computed data. It will enable searches for materials that exhibit desired properties and functions, to meet specific scientific or industrial requirements. Powerful **visualisation** and virtual-reality tools, offering multi-level, multi-dimensional navigation of the data will be developed and made available. Furthermore, the CoE's scientists will devise novel tools that can identify hitherto-unknown structure and trends in the large chemical compound space – an important tool for identifying promising new materials. These actions will help to identify new physical phenomena; they will advance materials science and engineering, and may yield novel technological devices and products.

Prof. Scheffler, the coordinator of the NOMAD CoE, comments: *"We are part of the cecamⁱ and Psi_kⁱⁱ community. These two organisations do an excellent job of linking scientists together. However, the integration of electronic-structure theory for materials and databases of computational materials science data, remains a major challenge. In NOMAD, we will combine big data and tools. Such an integration will make it easier for academic research and industrial actors to find, and to benefit from, materials science information which is directly relevant to their problems and opportunities."*

Please, find more information at <http://NOMAD-CoE.eu>

The NOMAD CoE partners are:

Max-Planck-Gesellschaft

King's College London

Humboldt-Universität zu Berlin

University of Cambridge

University of Barcelona

Aalto University, Helsinki

Technical University of Denmark, Lyngby

Leibniz-Rechenzentrum, Garching

CSC - IT Center for Science, Helsinki

Barcelona Supercomputing Center

Pintail Ltd

Prof. Matthias Scheffler, Fritz Haber Institute, Berlin (coordinator)

Stefan Heinzl, Max Planck Computing and Data Facility, Garching

Prof. Angel Rubio, Institute for the Structure and Dynamics of Matter, Hamburg

Prof. Alessandro De Vita

Prof. Claudia Draxl

Prof. Daan Frenkel

Prof. Francesc Illas

Prof. Risto Nieminen

Prof. Kristian Sommer Thygesen

Prof. Arndt Bode

Dr. Kimmo Koski

Dr. Jose Maria Cela

Ciaran Clissmann

ⁱ CECAM is a European organization devoted to the promotion of fundamental research on advanced computational methods and to their application to important problems in frontier areas of science and technology, in physics and chemistry of condensed matter: <http://www.cecam.org/>.

ⁱⁱ Psi_k is a Europe-based, worldwide network of researchers working on the advancement of first-principles computational materials science. <http://psi-k.net/>