

[BSC contributes to drive standardization and comparability in material science data](#)



Researchers from the Computer Applications department at Barcelona Supercomputing Center (BSC) contributed to the organization of the [CECAM](#) workshop "Towards a Common Format for Computational Materials Science Data". The workshop covered topics such as a common data format including a library and API, a common representation of important data, and ways of making results comparable. Amongst the attendants were representatives of more than 20 leading material science simulation packages (codes).

The workshop has taken place in the framework of the new Center of Excellence (CoE) '[Novel Materials Discovery Laboratory](#)' (NOMAD) which develops a Materials Encyclopedia and Big-Data Analytics tools for materials science and engineering.

CASE Department Director, José María Cela, states: “Standardization amongst material science simulation codes is an ambitious undertaking. Its complexity stems from conceptual differences between codes as well as historical developments. The outcome of this workshop is beneficial for code development in a wide range, and a basic ingredient for projects like the NOMAD Laboratory. The support of two large initiatives, CECAM and NOMAD, and the large amount of contributing codes ensure a rich outcome and impact of this effort.” 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 are enormous.

NOMAD will develop a Materials Encyclopedia 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.

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 super-computing centres. The project is funded for an initial three years, for almost 5 million euro, under the EU’s Horizon 2020 programme.

<http://nomad-coe.eu> | <https://twitter.com/NoMaDCoE> | <https://www.facebook.com/nomadCoE>

About BSC

Barcelona Supercomputing Center (BSC) is the leading supercomputing centre in Spain. It specialises in High Performance Computing (HPC) and its mission is two-fold: to provide infrastructure and supercomputing services to European scientists, and to generate knowledge and technology to transfer to business and society.

BSC is a Severo Ochoa Center of Excellence and a first level hosting member of the European research infrastructure PRACE (Partnership for Advanced Computing in Europe). BSC also manages the Spanish Supercomputing Network (RES).

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