# NoMaD: The Novel Materials Discovery Laboratory

## Description

Essentially every new commercial product, be they smart phones, solar cells, batteries, transport technology, artificial hips, etc., depends on improved or even novel materials. Computational materials science is increasingly influential as a method to identify such critical materials for both R&D. Enormous amounts of data, precious but heterogeneous and difficult to access or utilise, are already stored in repositories scattered across Europe.

The NoMaD CoE will open new HPC opportunities by enabling access to this data and delivering powerful new tools to search, retrieve and manage it. NoMaD will foster sharing of all relevant data, building on the unique CECAM, Psi-k and ETSF communities, putting Europe ahead of materials science in other continents. Unprecedented, already initialised networking with researchers, with industry, with students and with other stakeholders will guarantee relevance and end-user value. NoMaD will become a crucial tool for atomistic simulations and multi-scale modelling in the physical, materials, and quantum-chemical sciences. This field is characterised by a healthy but heterogeneous eco-system of many different codes that are used at all HPC centers worldwide, with millions of CPU hours spent every day, some of them at petascale performance. NoMaD will integrate the leading codes and make their results comparable by converting (and compressing) existing inputs and outputs into acommon format, thus making these valuable data accessible to academia and industry: NoMaD will develop big-data analytics for materials science. This will require novel algorithms, e.g., for statistical learning based on the created materials encyclopedia, offering complex searches and novel visualisations. These challenges exploit the essential resources of our HPC partners. Without the infrastructure and services provided by the NoMaD CoE, much of the information created with the above mentioned petascale (towards exascale) computations would be wasted.

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