NOMAD2: Novel Materials Discovery

Description

Predicting novel materials with specific desirable properties is a major aim of ab initio computational materials science (aiCMS) and an urgent requirement of basic and applied materials science, engineering and industry. Such materials can have immense impact on the environment and on society, e.g. on energy, transport, IT, medical-device sectors and much more. Currently, precisely predicting complex materials is computationally infeasible. NOMAD2 will develop a new level of materials modelling, enabled by upcoming HPC exascale computing and extreme-scale data hardware. In close contact with the R&D community, including industry, we will

- develop exascale algorithms to create accurate predictive models of real-world, industrially-relevant, complex materials.
- provide exascale software libraries for all code families (not just selected codes); enhancing today's aiCMS to take advantage of tomorrow s HPC computing platforms
- develop energy-to-solution as a fundamental part of new models.

This will be achieved by developing novel artificial-intelligence (AI) guided work-flow engines that optimise the modelling calculations and provide significantly more information per calculation performed; offer extreme-scale data services (data infrastructure, storage, retrieval and analytics/AI); test and demonstrate our results in two exciting use cases, solving urgent challenges for the energy and environment that cannot be computed properly with today's hard- and software (water splitting and novel thermoelectric materials); train the next generation of students, also in countries where HPC studies are not yet well developed.

NOMAD2 is working closely together with POP, and it is synergistically complementary to and closely coordinated with the EoCoE, ECAM, BioExcel and MaX CoEs. NOMAD2 will push the limits of aiCMS to unprecedented capabilities, speed and accuracy, serving basic science, industry and thus society.

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