

Data-driven Applications towards the Engineering of functional Materials: an Open Network (DAEMON)

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Current environmental, geo-political, and socio-economic challenges in the EU stem from a dependence of key technologies on critical and non-renewable materials. Discovery and commercialisation of innovative functional materials is needed to e.g. address energy production, storage and resilience, de-carbonise our economy to preserve ecosystems and climate, and switch current technologies to ethical and sustainable materials choices.

Data science and machine learning (ML) have recently boosted materials research in these areas, but it is urgent to expedite development. The DAEMON COST Action will grow a cross-disciplinary and pan-European network, which builds capacity and promotes education and research coordination, with the goal to accelerate materials discovery in Europe by means of cutting-edge computational techniques and data-driven methods.

The objective of this Action is to develop, harmonise, and promote the exploitation of ML methods for functional materials design. For targeted advancement, the Action will build working groups around innovative ML approaches that hold the most potential for new discoveries, and integrate them with network members focused on immediate applications. The action will leverage the synergic expertise of theorists and experimentalists in material science, physical chemistry, condensed matter physics, and computer science. In the process, the Action will train a new generation of young European researchers in a multi-disciplinary and transferable array of data science methods, and unite the non-ITC and ITC teams in cutting edge developments. Dissemination events will promote immediate technology transfer to our industrial stakeholders, maximising impact and societal benefit.

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