



Scuola Internazionale Superiore
di Studi Avanzati

Supercomputers for super materials

Innovative materials with outstanding properties designed through ultrafast computers. SISSA is hosting the first of a series of meetings to discuss potential scenarios



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The perspectives are really exciting and the opportunities in technology “unconceivable” until a few years ago, according to the experts. **The leading role is played by new materials which are efficient, innovative and have extraordinary properties. Supercomputers that can do an incredible number of operations in a very short time, rather than laboratory tests, are used to design them.** Nowadays, through simulations, scientists are able to do virtual experiments, predicting the behaviour and properties of raw materials, and thus to design new ones, with original features. Many important surprises are yet to come.

To discuss the advancements and perspectives of this area, **some of the top scientists in the field will be meeting on 10 and 11 January 2017 at SISSA, Trieste, Italy.** The initiative is among the activities of MaX (www.max-centre.eu), the European Centre of Excellence that works at the frontiers of High Performance Computing (HPC) technologies, to enable the best use and evolution of HPC for materials research and innovation. The Centre is coordinated by the Nanoscience Institute of the National Research Council (CNR) in Modena and involves some of the most important research and computing centres in Italy – such as the International School for Advanced



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Studies (SISSA) and the International Centre for Theoretical Physics (ICTP) in Trieste and the Cineca Consortium in Bologna – and abroad.

«This is an important step in a fast expanding field» explains Professor Stefano Baroni of SISSA, one of the MaX managers and co-organizer of the meeting. **«Computers allow us to do millions of virtual experiments, checking properties, performance and features of the material through numerical simulations, instead of doing thousands of experiments in the laboratory to get a single good result. The gain in terms of efficiency, speed and saving is huge».**

This is a world that bridges the most advanced research with industry. In Trieste, scientists and entrepreneurs will have the opportunity to meet and discuss.

Indeed, many are the potential applications of this new materials in the technology sector.

Examples include batteries that are getting smaller, lighter, quickly rechargeable, and long-lasting and may be used in consumer electronics, from mobile phones to PC, as well as in new generation electric cars. Major advancements are expected in the field of renewable energy as well as in the environmental sector, with products that may reduce the greenhouse effect and thus help the fight against global warming. Pharmaceutical industries are developing therapies that are more and more effective and safe. Moreover, food industries are looking for new substances for processing and preservation that may guarantee product quality and taste as well as consumer health.

That's not all. The MaX meeting will be the first of a series of events in Trieste focused on the applications of supercomputing to materials science. From 12 to 14 January, researchers from all over the world will meet at ICTP for the 18th International Workshop on Computational Physics and Materials Science "Total Energy and Force Methods". Then, from 17 to 27 January, ICTP will host a workshop on "High-Performance & High-Throughput Materials Simulations using Quantum ESPRESSO", one of the most important computational codes for quantum simulations of materials, developed in Trieste and among the main tools of MaX scientists.

(Immagine: Pixabay)

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