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NCCR Materials' Revolution: Computational Design and Discovery of Novel Materials (MARVEL)

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Main Leading House ETH Lausanne

Head Prof. Nicola Marzari

ETH Lausanne STI IMX THEOS

Station 12, MXC 337, CH-1015 Lausanne

phone: +41 21 693 11 29; office: +41 21 693 11 28

nicola.marzari@epfl.ch

Brief portrait

Society is in need of new materials to rise to the energy and environmental challenges it faces today. New materials have often been a source of societal progress. Good examples include the synthesis of ammonia, which transformed food production, and the doping of silicon, which led to the digital revolution. Society now needs new materials, for example for collecting solar energy and storing it as fuel or in batteries to distribute it efficiently, for recovering heat, as well as for efficiently converting mechanical energy into electrical energy.

So far, the development of new materials has been based primarily on intuition and trial and error. The National Centre of Competence in Research (NCCR) "MARVEL" is leading a scientific and technological revolution, whereby discoveries and inventions will come from information and communication technologies (ICT). As a result they will progress not at the speed of the physical world but at that of the world of information. This new approach is made possible by simulations based on quantum mechanics. Ever-increasing computing capabilities make it possible to conduct multiple simulations in parallel.

The NCCR "MARVEL" wants to apply this ICT approach to materials in the fields of energy, electronics and pharmaceuticals. But this will only be possible if synergies between the different areas of knowledgeare developes, such as materials science, chemistry, physics and computer science, all disciplines in which Switzerland has long-established expertise.

Research network

