THE DIGITAL INFRASTRUCTURES FOR 21st-CENTURY SCIENCE

Nicola Marzari

Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), EPFL STI IMX THEOS, Station 9, CH-1015 Lausanne (Switzerland), nicola.marzari@epfl.ch, https://nccr-marvel.ch

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Materials simulations have become powerful and widespread tools for scientific discovery and technological innovation, with billions of euros spent worldwide every year in supporting the researchers deploying these simulations. Applications range from nanotechnology to planetary science, from additive manufacturing to fine chemicals, from semiconducting qubits to Li-ion batteries. Against this backdrop, it is remarkable how comparatively little we plan and invest as a scientific society in developing, supporting, validating and disseminating such a successful research paradigm. The needs and resulting benefits are many, and go from verifying and validating the quantum engines in widespread use, to optimizing their performance on complex architectures, lowering the adoption threshold by enhancing usability and reliability, and integrating data and simulation services. I'll contextualize this with the ongoing worldwide efforts and our own, dedicated to developing and supporting core quantum engines, the AiiDA and AiiDAlab environments needed to provide user-friendly automates simulations [1,2], and the Materials Cloud dissemination platform [3] for curated and raw FAIR data.

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