

## Seminar #10

October 16, 2020, 11:30 am

*The great acceleration in the design and discovery of novel materials*

**Nicola Marzari**

École Polytechnique Fédérale de Lausanne



Materials are at the core of our technological advances, and are needed to address many of our societal challenges: from energy to information, from food to medicine. I'll highlight the great strides made in the last few years in the design and discovery of novel materials, where computational simulations can now precede, streamline, or accelerate experiments. This acceleration is driven by the central paradigm of computational science (doubling performance every 14-16 months), combined with powerful and predictive quantum simulation techniques, and by the convergence of data mining and machine learning towards materials simulations. I'll also underscore the IT requirements needed to perform calculations in a reproducible, shareable, high-throughput mode, highlighting applications to novel two-dimensional materials and solid-state Li-ion conductors.



## Virtual DCMIC Seminar Series

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