

## **Nicola MARZARI**

Ecole Polytechnique Federal de Lausanne, EPFL  
National Centre for Competence in Research MARVEL  
Station 9, CH-1015 Lausanne  
SWITZERLAND

### **Computational materials discovery: good data vs big data**

#### Abstract:

I'll present our approach and case studies in the broad area of computational design and discovery of novel materials, with a special focus on novel two-dimensional materials and Li-ion solid-state conductors. In the process, I'll highlight the needs and the infrastructure we built to manage massive amounts of calculations arising from such efforts, ensure the full reproducibility and provenance of the data, and allow the entire community to access, share, and store reliable and robust computational workflows and the resulting curated and raw data.