

Physics-aware AI to engineer materials: from atoms to technological applications

Michele Simoncelli¹

¹*Department of Applied Physics and Applied Mathematics, Columbia University, New York (USA)**

The ongoing AI revolution is transforming how scientists understand, design, and engineer functional materials. This talk will focus on recent methodological advances that leverage physics-aware AI models to predict the microscopic quantum interactions among electrons and nuclei, which ultimately govern the properties and behavior of materials. In particular, we will show how these models can be trained using quantum-mechanical calculations and combined with physical theories to predict technologically relevant properties, including how materials transport electricity, heat^{1,2}, and light, as well as how they age when exposed to extreme conditions³. We will discuss how physics-based benchmarks from the atomistic to the macroscopic scale allow us to assess when models are predictive from the bottom up — that is, when they accurately predict macroscopic properties because they correctly describe the underlying atomistic physics — and to detect when apparently sensible macroscopic predictions instead arise from cancellations among microscopic errors⁴. We conclude by outlining open grand challenges, whose rigorous resolution has the potential to transform the design of materials for technologies ranging from solar cells to nuclear fusion reactors.

* michele.simoncelli@columbia.edu

- [1] M. Simoncelli, N. Marzari, and F. Mauri, *Physical Review X* **12**, 041011 (2022).
- [2] K. Iwanowski, G. Csányi, and M. Simoncelli, *Physical Review X* **15**, 041041 (2025).
- [3] M. Simoncelli et al., *Proceedings of the National Academy of Sciences* **122** (2025).
- [4] B. Póta, P. Ahlawat, G. Csányi, and M. Simoncelli, *Nature Communications* (2026).