Artificial Intelligence enabling disruptive 2D materials *design & engineering*

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Abstract
In this talk, I will discuss the emerging need to massively use and deploy Artificial Intelligence (AI) techniques in materials and devices design and engineering [1]. AI is not only accelerating our access to complex information and knowledge, but is invading all sectors of our scientific practices and industrial innovation strategies. I will first overview our journey into the research of innovative advanced materials (amorphous boron-nitride based compounds) using AI in the field of interconnects technologies, which has demonstrated the critical role of combining AI techniques with linear scaling quantum simulation algorithms [2] to achieve unprecedented simulation of electronic properties of models with multimillion atoms while keeping ab-initio accuracy. This is bringing a revolutionary paradigm shift in the way researchers and engineers can access hidden and deeper layers of information for interlinking structural features down to the atomic scale with ultimate material properties as well as device and technology performances across all industrial fields.

I will point towards the emerging revolution of fully describing as-grown materials with AI-driven reconstruction of digital models/twins with atomistic modelling (from polycrystalline graphene to semiconducting materials for qubits industry). This opens a tremendous capability to correlate in-depth atomistic-scale features of as-grown materials with resulting local and global chemical, physical and devices properties, offering reverse engineering and AI-driven co-piloting for industrial innovation strategies. Some illustration will be given on developing end-to-end workflows [2] serving as pathfinder for advanced nanoelectronics, thermal management in high-power devices, neuromorphic computing hardware and advanced spintronic technologies using 2D materials and beyond.

All research and technology fields are to be radically affected and transformed by this AI revolution in materials science and technology, which I will illustrate in particular among the variety of research fields pursued during a decade by the Graphene Flagship initiative (https://graphene-flagship.eu/) and now continued within the Innovative Advanced Innovative Materials initiative/partnership (www.iam-i.eu), which will shape the future of European and worldwide landscape for the ten years to come. New initiative like our ICN2-ICREA spinoff "Apeiron Intelligence" will contribute to boost the design of novel materials and devices and reinforce industrial competitiveness.

References

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