Artificial Intelligence for realistic modelling of electronic, thermal, optical and transport properties in **trillion atoms scale models** in complex forms of 2D Materials-based composites and amorphous compounds

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Abstract

Artificial Intelligence-based techniques have become critical to accelerate the innovation processes from material growth to characterization and properties prediction. Particularly challenging is the modelling of disordered (amorphous) materials, complex interfaces and random assemblies of (2D) materials which are mainly used today in applications.

In that perspective, complex forms of (reduced) graphene oxides and related composites as well as amorphous materials such as boron nitride (aBN) and “amorphous graphene” (aG) have recently become prominent materials for many different applications, notably due to their good properties such as thermal stability, mechanical properties, insulating behaviour, and ultralow dielectric constant in aBN (<2). Moreover, amorphous films are more suitable to large area deposition compared to clean hBN or graphene since they can be grown at low temperatures (about 400 ºC) and on various substrates [1-3]. However, their properties strongly depend on the nature and degree of disorder, which needs a well-defined metrics for benchmarking different materials. Having such metrics in place will allow to tune the properties and performance of these films during the fabrication for desired applications. In this context, revealing the relationship between fabrication strategies and the material properties of the film is also crucial.

Capturing the key features of the amorphous nature of materials requires theoretical characterization to understand how material properties change with the microstructure. Since simulations of amorphous materials need large structural models, density functional theory (DFT) is not a suitable tool despite the high accuracy it offers. On the other hand, molecular dynamics (MD) simulations with empirical interatomic potentials require much less computational cost; however, they can turn out to be not accurate enough to correctly describe the local environment of amorphous materials. Machine learning-driven interatomic potentials (ML-IP) can describe the local environment with a similar accuracy to DFT and at a much lower cost [4,5]. Here, we introduce Gaussian approximation potentials (GAP) for atomistic simulations of aBN incorporating different contaminators and doping materials, which are trained on a large dataset of atomic structures generated by DFT calculations [6-8]. We will present a systematic analysis to screen out possible realistic morphologies as a function of growth parameters, such as temperature, quenching rate, and the presence of a dopant, and their corresponding material properties using GAP-driven MD simulations. The extensive simulations of a large quantity of possible structures presented here can guide experimental research and provide trends of scaling behaviour as a function of experimentally controllable parameters. The impact of amorphousness on dielectric properties will be also discussed for aBN and aG in the light of recent breakthroughs and claims [9,10].

We also present AI-driven computational workflows that could revolutionize advanced materials design and engineering, in which the automated building of structural and electronic models and their implementation into our in-house linear scaling computational algorithms (www.lsquant.org) enables the simulation of electronic, optical, transport properties in disordered models of materials containing up to the trillion atoms scale while keeping the accuracy of ab-initio approaches. These workflows will be designed to boost the innovation in a variety of technologies and applications in concertation and partnerships with industries.

References

[1] Hong, S et al. Nature 582, 511–514 (2020).
[2] Glavin, N. R., et al., Adv. Func. Mat. (2016).
[3] Chen, C. Y., et al., arxiv: 2312.09136 (cond-mat).
[4] Unruh D. et al. Physical Review Materials 6, 065603 (2022).
[5] Deringer, VL. and Csányi, G. Physical Review B 95, 094203 (2017).
[6] Kaya, O., et al. Nanoscale Horizons 8, 361–367 (2023).
[7] Kaya, O. et al. J. Phys. Materials 7, 025010 (2024).
[8] Kaya, O. et al. arXiv:2402.01251 (cond-mat).
[9] Th. Galvani et al. Journal of Physics: Materials 7 (3), 035003 (2024); arXiv:2403.11924 (cond-mat).
[10] Th. Galvani, O. Kaya, S. Roche, unpublished