From Order to Disorder: Assessing Thermal Properties in Amorphous Graphene with Machine Learning-Driven Simulations

H. Shoaib[1], S. Huberman[1]

[1]*Department of Chemical Engineering, McGill University, Montreal, Quebec H3A 0C5, Canada*

hassan.shoaib@mail.mcgill.ca, samuel.huberman@mcgill.ca

The study of thermal properties in amorphous graphene presents unique challenges and opportunities for advancing material science and engineering. Traditionally, investigations into the thermal properties of amorphous carbon materials have relied on empirical potentials designed for pristine graphene, stretching these models beyond their intended domain of applicability [1]. This research seeks to overcome these limitations by utilizing efficient and high fidelity machine learning interatomic potentials (MLIP).

Achieving an accurate yet computationally efficient representation of the potential energy surface (PES) for materials is highly important. While methods like density functional theory (DFT) offer detailed and transferable insights by explicitly accounting for the electrons in a system, their applicability is hampered by poor scalability with increasing system size, confining their practical use to relatively small systems and limiting the duration of simulations. A critical examination of existing methodologies in the classical route reveals that while current MLIPS for carbon materials offer a high degree of accuracy, their utility in the study of amorphous graphene is hindered by substantial computational demands [2]. This limitation is particularly pronounced when dealing with large, disordered systems where the computational expense can become prohibitive.

Addressing this gap, our work seeks to use a MLIP for amorphous graphene that has excellent scalability, such as potentials based on the allegro framework, a strictly local equivariant deep neural network inter-atomic potential [3] that can be accelerated using GPUs. In the realm of molecular dynamics (MD), the advent of GPU parallelization has been a game-changer, significantly enhancing computational capabilities. The scalability is crucial for our study, which involves the intricate thermal properties of amorphous graphene structures, known for their computational intensity due to disorder. The generation of amorphous graphene structures, through the incorporation of Stone-Wales defects via a Monte Carlo algorithm, will enable a controlled exploration of disorder in carbon-based materials. The interatomic potential will be applied to a large-scale amorphous structure, with its results benchmarked against those derived from empirical potentials.

By adopting this approach, our study not only adeptly navigates the computational hurdles associated with the intricate nature of amorphous graphene but also sets a new precedent for the accurate, efficient investigation of thermal properties in disordered carbon materials. Our findings aim to contribute to a deeper understanding of heat transfer mechanisms in amorphous graphene, paving the way for the development of advanced materials with tailored thermal properties for use in a wide range of applications, from electronics to energy storage.

1. Carbon: 2D graphene, 1D nanotubes, and 0D quantum dots.

References

[1] Bazrafshan, S., & Rajabpour, A. (2017). Thermal transport engineering in amorphous graphene: Non-equilibrium Molecular Dynamics Study. International Journal of Heat and Mass Transfer, 112, 379–386.

[2] Rowe, P., Deringer, V. L., Gasparotto, P., Csányi, G., & Michaelides, A. (2020). An accurate and transferable machine learning potential for carbon. The Journal of chemical physics, 153(3), 034702.

[3] Musaelian, A., Batzner, S., Johansson, A. et al. Learning local equivariant representations for large-scale atomistic dynamics. Nat Commun 14, 579 (2023).