Ab initio modelling of nitrogen-graphite scattering with neural-network molecular dynamics

Samuel Cajahuaringa[1],
Davide Bidoggia[1], Enrico Smargiassi[1], Antimo Marrazzo[2], and Maria Peressi[1]
[1]*Università degli Studi di Trieste, via A. Valerio 2, Trieste 34127, Italy*
[2]*Scuola Internazionale Superiore di Studi Avanzati, via Bonomea 265, Trieste 34136, Italy*
oscarsamuel.cajahuaringamacollunco@units.it

Abstract

Developing materials with reduced drag forces are crucial for many applications, from aerospace technologies to transportation industry. The accurate description of gas-surface interactions plays a pivotal role in this endeavor. Molecular dynamics simulations offer a powerful tool for understanding gas-surface interactions. By comparing molecular dynamics with gas beam experiments, it is possible to validate theoretical models for the gas-surface interaction. In this work, we employ molecular dynamics simulations with neural-network potential[1] trained on ab initio simulations to study molecular nitrogen impinging on multilayered graphene at different incident angles. Our results using neural network potentials display better agreement with available beam scattering experiments when comparison with classical force fields[2]. Furthermore, we calculate accommodation coefficients, quantifying energy and momentum transfer between gas molecules and surfaces, that play a crucial role in the study of drag[3].

Acknowledgments: Authors acknowledge support through the Innovation Grant "ASGARD - Atomistic Simulations of damage, adhesion and drag reduction of graphene-based coatings" from the ICSC—Centro Nazionale di Ricerca in High Performance Computing, Big Data and Quantum Computing, which was funded by the European Union: Next-GenerationEU (CUP Grant No. J93C22000540006, PNRR Investimento No. M4.C2.1.4).

References

[1] F. Pellegrini, S. de Gironcoli, E. Küçükbenli, arXiv:2405.08137 (2024).
[2] N. Andric, P. Jenny, Phys. Fluids, 30 (2018), 077104.
[3] N. A. Mehta, D. A. Levin, *J. Thermophys. Heat Transf*. 31(4) 2017, 757-771.

Figures

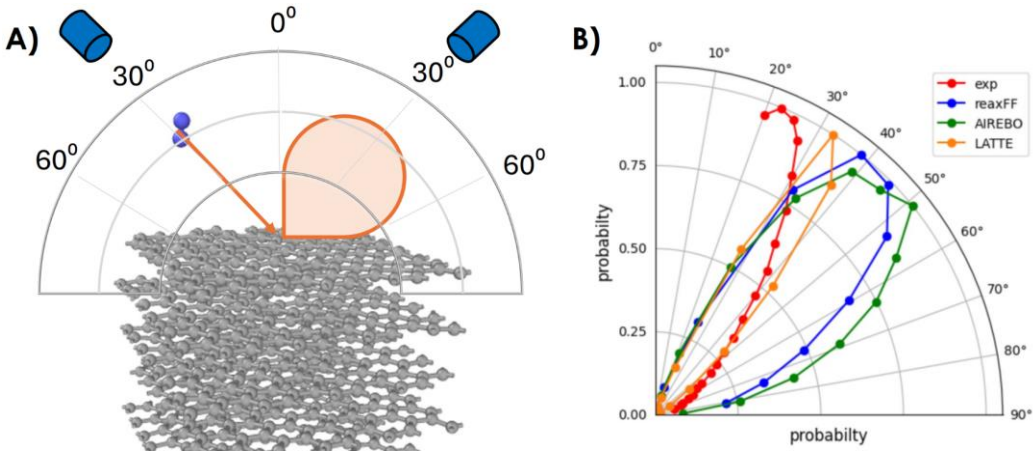

Figure 1: A) Schematic representation of nitrogen gas scattering on graphite. **B)** Angular distribution of scattering angles for experiments (•), classical force fields reaxFF (•) and AIREBO (•) [2] and LATTE neural-network potential (•) [1].