High-Dimensional Atomistic Neural Network Potential to Study the Alignment-Resolved O_2 Scattering from Highly Oriented Pyrolytic Graphite.

A. Rivero Santamaría[1*], M. Alducin [1,2], R. Díez Muiño [1,2] and J. I. Juaristi[1,2,3]

[1] *Donostia International Physics Center DIPC, San Sebastián, Spain*
[2] *Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), San Sebastián, Spain*
[3] *Departamento de Física de Materiales, Facultad de Químicas (UPV/EHU), San Sebastián, Spain*

*Presenting Author E-mail: arivero@dipc.org

The main shortcoming of Ab Initio Molecular Dynamics (AIMD) simulations is the statistical accuracy, since due to their high computational cost, a relatively small number of trajectories can be performed. In the last few years, the irruption of machine learning algorithms has allowed to construct High Dimensional Atomistic Neural Network Potential Energy Surfaces (ANN-PESs), that based in atomistic neural networks[1], can be used to perform molecular dynamics studies taking into account all the degrees of freedom of the system, allowing high-quality simulations on full-dimensional analytical PESs with a low computational cost.

This work is focused on developing a full dimensional ANN-PES using the open source software package, the atomic energy network (aenet) code[2] feed with the DFT data obtained in our previous AIMD calculations[3] on the alignment dependent scattering of O_2 from highly oriented pyrolytic graphite (HOPG). The results obtained in the validation step demonstrate the ability of the ANN-PES to reproduce accurately the interaction of O_2 with the HOPG surface. The use of the obtained PES allows us to perform much more trajectories at different initial conditions, significantly increasing the statistic of our calculations and allowing a more accurate description of the relevant dynamical magnitudes in the scattering process. The results of our simulations are in overall agreement with our previous AIMD calculations[3] and with recent experimental observations[4], showing a weak alignment dependence in the angular distributions and a clear energy transfer dependence on the initial alignment of the O_2 molecule.

References

[1] Behler, J.; Parrinello, M. Phys. Rev. Lett. 98, 146401 (2007)
[2] Artrith, N.; Urban, A. Comput. Mater. Sci,114, 135–150 (2016)
[3] Rivero Santamaría, A.; Alducin, M.; Diez Muino, R.; Juaristi, J. I. J. Phys. Chem. C, 123, 51, 31094-31102 (2019)
[4] Kurahashi, M.; Takahiro, K, Phys. Rev. B. 99, 045439 (2019)