How Water Tunes Quantum Transport in Nanoporous Graphenes: An Artificial Intelligence Approach

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Abstract

The structure and dynamical behaviour of water confined at, or in, nanostructures is a topic central to many fields from biology to emerging electronics such as carbon nanostructures. Nanoporous graphenes (NPGs) containing periodic nanoscale pores with specific topologies have emerged as a rising star in carbon-based nanoelectronics, however, their interaction with ambient water still remains an open question. Understanding this interaction is challenging, as atomic-scale experiments are difficult, and ab-initio mechanistic studies are prohibitively expensive. To tackle this fundamental challenge, we develop both ‘black-box’ and physics-informed ‘grey-box’ machine learning (ML) models that unravel the complex structure-bandgap relationships of pristine NPG and hybrid nitrogen-doped porous graphene (h-NPG) under dynamic aqueous environments. Trained on ab-initio data, our interpretable ML models, predict bandgaps for diverse structural ensembles of NPG with near-DFT accuracy (R^2 ~ 100%, MAE ~ 0.002 eV), while preserving underlying physical principles and significantly reducing computational cost. To shed light on the structure and chemistry of NPGs aqueous systems at a molecular level, we further perform a detailed analysis of structural, electronic and transport properties and find them highly sensitive to the spatial arrangement of water molecules, leading to configuration-dependent bandgaps. This way, the present study provides deep mechanistic insights into wet nanoporous electronics, and open pathways for the rational design of humidity-responsive nanoelectronic devices.

References

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Figures

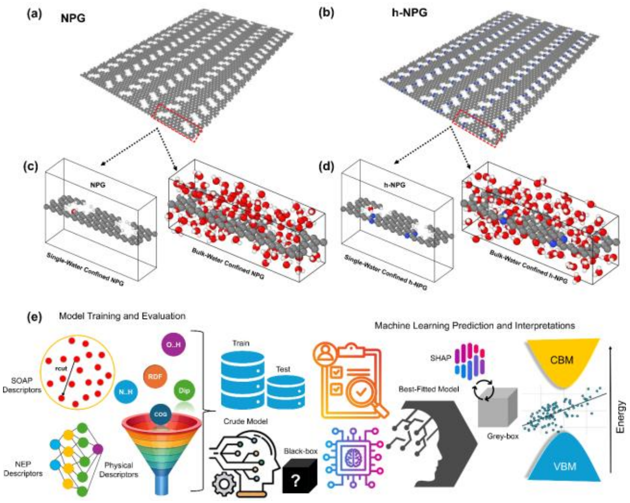

Figure 1. Schematic illustration of (a) pristine (NPG) and (b) nitrogen-doped (h-NPG) nanoporous graphenes; relaxed geometries of single-water and bulk-water confined (c) NPG and (d) h-NPG unit cells; (e) model training and evaluation stage, where structural descriptors—including SOAP, NEP, and physics-based features—are extracted to capture the relationship between atomic configurations and bandgap energies and used to train and test multiple machine-learning models. In the prediction and interpretation stage, initially trained (crude) models are further optimized to identify the best-fitting grey-box model. The final model is interpreted using SHAP analysis and applied to predict configuration-dependent bandgap energies for previously unseen nanoporous graphene structures.