Study of the IV characteristics for quantum-confined bio-molecular nanostructure: DFT and Machine Learning based combined framework

ID: ORL05
Oral Talk
Aug. 24, 15.30 - 15.50

Debarati Dey Roy,[1,†] Pradipta Roy,[2,†] and Nguyen Thanh Tien[3]

[1] *Department of Electronics & Communication Engineering, B. P. Poddar Institute of Management & Technology. 137, V. I. P Road, Kolkata-700052, West Bengal, India*

[2] *Dept. of Computer Application, Dr. B. C. Roy Academy of Professional Courses. Fuljhore, Jemua Road, Durgapur-713206. West Bengal, India*

[3] *College of Natural Sciences, Can Tho University, Campus II, Can Tho University, 3/2 street, Ninh Kieu District, Can Tho City, Vietnam*

Email: debaratidey24@gmail.com, pradiptoroy@gmail.com

Keywords: Machine Learning, DFT, Artificial Intelligence, I-V Characteristics, Conductivity

Machine Learning (ML) application is a boon for electronic structure prediction. The combined framework of Density Functional Theory (DFT) and ML algorithms makes the prediction work easier for Nanotechnologists. The algorithmic approach of ML towards the electronic structure theory permits the prediction of electronic characterization for molecular models. The time-consuming task of electronic structural prediction for quantum confinement into nano-dimension systems became easier with the introduction of Artificial Intelligence (AI). This article presents the best-fitted prediction model for the quantum-confined Adenine molecular nanoribbon using DFT and ML-based combined framework. Our framework introduces an algorithm to predict electronic characteristics, such as the current-voltage response graph and the graphical presentation of the conductivity with high accuracy. The regression learner will predict the graphical representation of various electronic characteristics of the quantum-confined bio-inspired nanostructure. A learnable real-space Hamiltonian procedure and k-point sampling are introduced to extract the information and feed it into the machine to train it to create a future prediction model for this quantum-confined Adenine nanoribbon. The best-fitted regression learner provides approximately 85% accuracy for this quantum-confined Adenine nanoribbon structure. This framework provides a faster and more accurate prediction model for electronically characterizing the quantum-confined bio-inspired nanoscale structure [1-4].

References

1. D. D. Roy and D. De, "Predicting model of I–V characteristics of quantum-confined GaAs nanotube: a machine learning and DFT-based combined framework", J. Comput. Electron. **22**, 999-1009 (2023).
2. D. D. Roy, P. Roy, and D. De, "Machine learning and DFT-based combined framework for predicting transmission spectra of quantum-confined bio-molecular nanotube". J. Mol. Model. **29**, 338 (2023).
3. D. Dey, P. Roy, and D. De, "Electronic characterisation of atomistic modelling based electrically doped nano bio p-i-n FET", IET Comput. Digit. Tech. **10**, 273-285 (2016).
4. O. T. Hofmann, E. Zojer, L. Hörmann, A. Jeindl, and R. J. Maurer, "First-principles calculations of hybrid inorganic–organic interfaces: from state-of-the-art to best practice", Phys. Chem. Chem. Phys. **23**, 8132-8180 (2021).