

Comparative Analysis of Classical and Quantum Machine Learning Models for Nanomaterial Property Classification



Chaima Gharbi¹², Wejden Gazehi¹², Rania Loukil¹², Mongi Besbes¹²

¹Higher Institute of Information and Communication Technologies, University of Carthage, Tunis, Tunisia

²Laboratory of Robotics, Informatics and Complex Systems, ENIT, University of Tunis El Manar, Tunis, Tunisia

The accurate prediction and classification of nanomaterial properties constitute essential prerequisites for the rational design and systematic optimization of nanocomposites in chemical engineering contexts. The present study investigates the application of classical and hybrid quantum--classical machine learning frameworks to establish quantitative structure--property relationships between nanoparticle descriptors and their corresponding physicochemical attributes. Four computational approaches are systematically examined: K-Nearest Neighbors (K-NN), Decision Tree (DT), Random Forest (RF), and a novel Quantum Feature Random Forest (QFRF) architecture for nanoparticle property classification.

Model performance is rigorously assessed using standard statistical metrics, including classification accuracy, Mean Squared Error (MSE), Root Mean Squared Error (RMSE), F1-score, and precision. Comparative analysis reveals that the hybrid QFRF framework exhibits markedly superior predictive capability relative to conventional machine learning methods, achieving a classification accuracy of 91.78\% with substantially reduced prediction errors (MSE = 0.2556, RMSE = 0.5055). The concomitant improvements in F1-score and precision further demonstrate enhanced model robustness and reliability.

These results establish that the incorporation of quantum-derived feature representations into ensemble learning architectures leads to significant improvements in nanomaterial property prediction. From a chemical engineering standpoint, this data-driven computational framework provides a robust and efficient methodology for nanomaterial characterization, optimization, and inverse design, thereby facilitating the accelerated development of advanced nanocomposites and streamlining materials discovery pipelines.

Biography:

Chaima Gharbi received her Baccalaureate degree in 2020. She obtained her Bachelor's degree in Telecommunications in 2023 from the Higher Institute of Information and Communication Technologies, University of Carthage, Tunisia. She then completed a Research Master's degree in Data Science and Intelligent Services in November 2025 at ISTIC. Currently, she is a first-year PhD student at the École Polytechnique de La Marsa. Her research is at the intersection of quantum physics and artificial intelligence, with a strong focus on machine learning and deep learning techniques. Her research interests encompass nanotechnology and artificial intelligence, particularly nanoparticle classification using advanced AI-based models.