Leveraging Machine Learning and Statistical Methods for Predicting Excitons in Two-Dimensional Materials

M. Szyszko[1], M. E. Marchwiany[2], T. Woźniak[1] and M. Birowska[1]

[1] *University of Warsaw, Faculty of Physics, 00-092 Warsaw, Pasteura 5, Poland*
[2] *Interdisciplinary Centre for Mathematical and Computational Modelling (ICM), University of Warsaw, Pawińskiego 5a, 02-106 Warsaw, Poland*

Atomically thin semiconducting van der Waals (vdW) layered materials are potentially interesting candidates for various applications in opto-electronics, due to extremely strong light-matter interactions as a result of the enhanced excitonic effect in two dimensions. Excitons play a pivotal role, influencing optoelectronic phenomena and device performance [1]. However, predicting excitonic behavior in 2D materials remains a complex challenge due to the intricate interplay of various material parameters such as electronic features and structural configurations, as well as dielectric environment and substrate.

This work presents our ongoing research efforts aimed at harnessing machine learning (ML) and statistical learning methods to predict excitons in 2D materials. By leveraging advanced computational techniques and vast datasets [2-3], we seek to unravel the underlying patterns governing excitonic behavior and enhance our understanding of their fundamental properties. Our approach involves the integration of diverse datasets encompassing material characteristics, structural parameters, and excitonic properties obtained through advanced spectroscopic techniques and computational simulations. Through meticulous data preprocessing and feature engineering, we strive to extract meaningful insights and establish correlations between input variables and exciton behavior. The core of our methodology revolves around the development and optimization of predictive models using state-of-the-art ML algorithms, such as random forests. By training these models on labeled datasets and employing rigorous cross-validation techniques, we aim to achieve robust predictions of excitonic properties with high accuracy and reliability.

[1] Zheng, X., Zhang, X. Excitons in two-dimensional materials. *Advances in Condensed-Matter and Materials Physics-Rudimentary Research to Topical Technology*, (2019).
[2] Sten Haastrup, Mikkel Strange, et al. 2D Materials **5**, 042002 (2018).
[3] M. N. Gjerding, A. Taghizadeh, A. Rasmussen, et al. 2D Materials **8**, 044002 (2021).