Advancing biomaterials modeling: development of physically inspired machine learning force fields

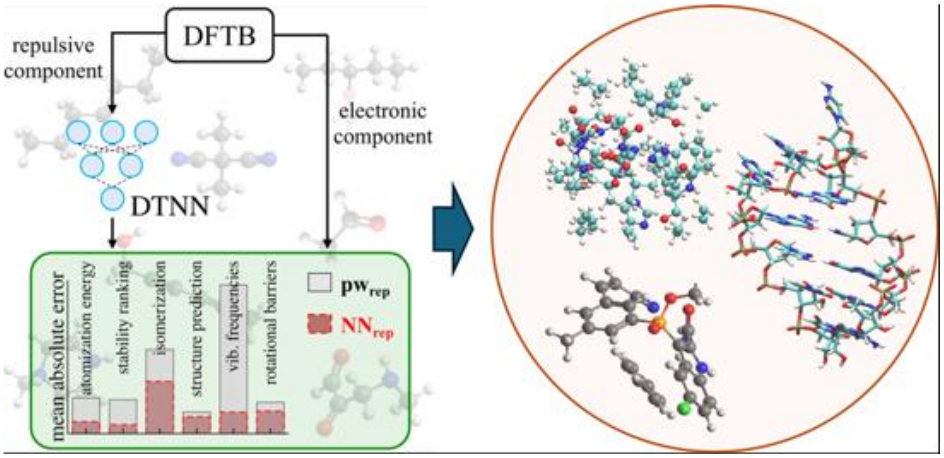

Figure modified from Ref. [*Phys. Chem. Lett.* 11, 16, 6835–6843, (2020)].

The modeling of **biomaterials** plays a pivotal role in the modern medicine discovery pipeline, as it mitigates the cost, time, and resources required to screen novel candidates for biological targets and gene technology. Hence, it is crucial to accelerate these simulations using **machine learning (ML)** and **quantum mechanics (QM)**, developing a comprehensive computational method capable of accurately investigating biological processes and functions that are challenging for current simulation methods.

The **GOAL** of this thesis is to develop ML force fields for biomaterials to investigate their thermodynamics and structural properties based on a quantum-mechanical description of inter-and intramolecular interactions. The insights gained through the analysis of QM data will be validated using classical MD simulations and experimental data, when available.

References

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