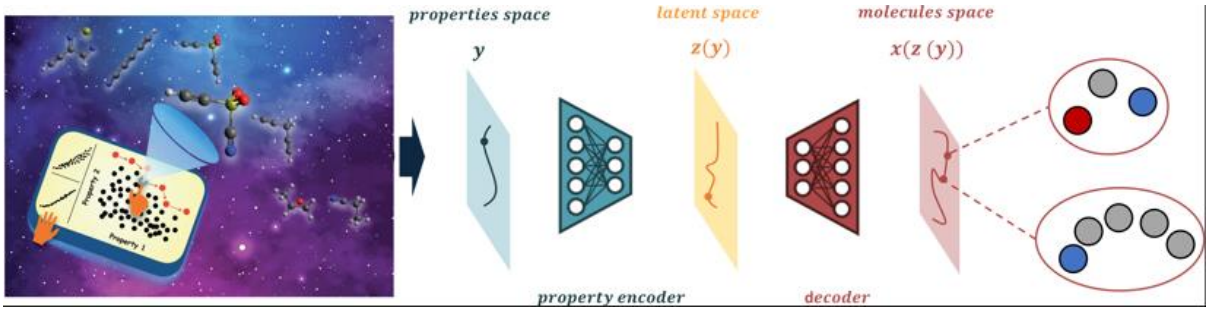
Generative models for the computational design of quantum materials



Figures extracted from Ref. [*Chem. Sci.* 14, 10702-10717, (2023)] and Ref. [*Nat. Commun.* 15, 6061, (2024)].

The discovery and optimization of **quantum materials** can be accelerated thanks to the marked advancements in quantum and statistical methods, their implementation in advanced software, as well as the seemingly never-ending improvement in computer hardware. Thus, computer-driven molecular design combines the principles of chemistry, physics, and artificial intelligence to identify compounds with tailored properties. While **quantum-mechanical** (QM) methods, coupled with **machine learning**, already offer a direct mapping from 3D molecular structures to their properties, effective methodologies for the inverse mapping in diverse chemical space remain elusive. Notable advancement in this area is the implementation of **generative AI frameworks** to design novel compounds with desired physicochemical properties.

The **GOAL** of this thesis is to use quantum mechanics to explore chemical spaces spanning low-dimensional materials, gaining insights into structure-property and property-property relationships. The student will then develop generative models for the targeted design of quantum materials with specific functionalities.

References

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

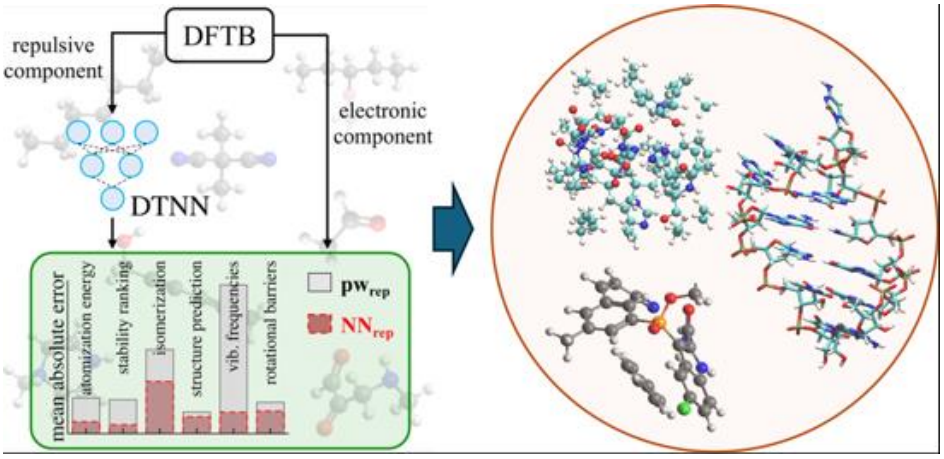

Figure modified from Ref. [*Phys. Chem. Lett.* 11, 16, 6835–6843, (2020)].

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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