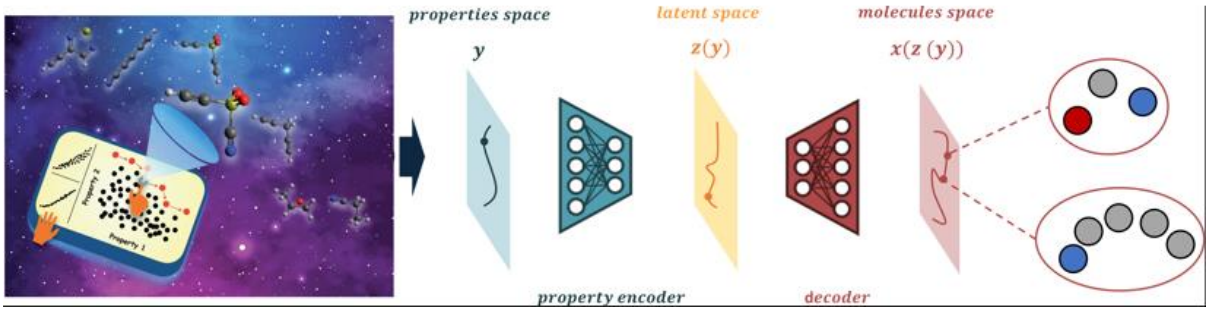
Generative models for the computational design of quantum materials



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

Anstine, D. M. & Isayev, O. Generative models as an emerging paradigm in the chemical sciences. J. Am. Chem. Soc. 145, 8736–8750 (2023).

A. Fallani, L. Medrano Sandonas, A. Tkatchenko. Inverse mapping of quantum properties to structures for chemical space of small organic molecules. Nat. Commun. 15, 6061, (2024).

L. Medrano Sandonas, J. Hoja, B. G. Ernst, A. Vazquez-Mayagoitia, R. A. DiStasio Jr., A. Tkatchenko. "Freedom of design" in chemical compound space: towards rational in silico design of molecules with targeted quantum-mechanical properties. Chem. Sci. 14, 10702-10717, (2023).