Machine Learning for Medicine: Accelerating Metadynamics of Supramolecular Host-Guest Complexes for Therapy and Imaging

Contacts:

Prof. Angela Casini (Chemistry, NAT), angela.casini@tum.de;

Prof. Alessio Gagliardi (Electrical and Computer Eng., CIT), alessio.gagliardi@tum.de;

Position: 1 year funded 100% TV-L E13 position (German system). The position will be shared between the two groups of Prof. Angela Casini and Prof. Alessio Gagliardi at the Technische Universität München.

Requirements: we hire a PostDoc with expertise in (i) atomistic modelling (Density Functional Theory, Molecular Dynamics, ab-initio Molecular Dynamics, Metadynamics) and (ii) machine learning (mostly deep learning algorithms) to develop new data driven methods for metadynamics to accelerate the optimization of supramolecular materials (metallacages) for medical applications.

Project: In the context of 3-dimensional porous supramolecular materials (metallacages) computational methods hold promise to accelerate the challenging process of designing and optimizing their host-guest chemistry and encapsulation properties. Amongst the possible atomistic simulation approaches, metadynamics (metaD) has proven very powerful. However, the choice of high level chemical descriptors, i.e. the collective variables (CVs), to accelerate the numerical computation is not trivial for complex systems. To automate the process of CVs identification, we apply here different machine learning algorithms to the metaD simulation of metallacages designed for biomedical applications, including drug delivery, imaging and therapy.