Optimized Supramolecular Materials for Sustainable Energy Solutions and Regenerative Medicine powered by Machine Learning

Prof. Alessio Gagliardi

Electrical and Computer Engineering, Simulation of Nanosystems for Energy Conversion,

Technische Universität München

The present PhD position is part of a novel project: the TUM Innovation Network for Artificial Intelligence powered Multifunctional Material Design (ARTEMIS)[1]. The project addresses critical challenges of Data-Science-driven Materials Chemistry & Engineering by coalescing two distant areas of research under the roof of Machine Learning (ML): (A) The exploration of materials facilitating *storage and release of energy in and from chemical bonds,* thus providing **sustainable energy solutions**, and (B) the development *tailored multifunctional materials* for **regenerative medicine**. There is deep, latent similarity and homeomorphism of the research and experimental design challenges at the level of Materials Chemistry between these two areas. Specifically, we will investigate a novel family of **Supramolecular (hybrid) Materials** (e.g.: Metal-Organic Frameworks, MOFs; Organic Supramolecular Polymers, OSPs; Derived Hybrid Materials, DHMs). These materials are bearing great potential for innovative applications in **electrocatalytic water splitting for hydrogen production**, **for guided tissue regeneration and for 'smart' coating of medical implants**. The selected materials space is ideally suited for ML-based discoveries. ML is emerging as a third path to boost materials discovery besides 'theory & numerical simulations' and 'experiments & characterization'. However, to reach the same maturity that has been achieved in other areas of Data Science, ML needs to overcome distinct challenges to develop new highly performing machines specifically designed for Materials Chemistry. Thus, based on systematic and rational feedback from experiment into algorithm and database development and *vice versa*, ML will power our materials discovery and experimental design.

The PhD position will work in tight connection with several other PhD students and will be supervised by a PostDoc. His topic will be the development and testing of datasets using numerical methods (Density Functional Theory, Monte Carlo, Molecular Dynamics) for the developed machines, in particular Graph Neural Networks. He will mostly concentrate on supramolecular polymers and MOF for host-guest chemistry.

Contact: alessio.gagliardi@tum.de

Required skills: programming, machine learning, material science.

Contract Type/Length: 100% E13 position (3 years).

[1] https://www.tum.de/en/studinews/issue-032015/show/article/36529/