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

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The present topic 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.

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Required skills: programming, machine learning, material science.

Contract Type/Length: 100% E13 position (2 years).