

Computational design of nature-learned sustainable materials

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Abstract: Artificial intelligence, and particularly machine learning, is transforming our ability to predict chemical properties, discover new molecules, and accelerate atomistic simulations. We leverage this emerging paradigm to design and simulate nature-inspired materials, focusing on sustainable building blocks derived from biomass waste and non-critical resources. Our research focuses on elucidating structure–property relationships, as well as the assembly pathways and degradation mechanisms of biomolecules and biomass-derived materials. By integrating computational chemistry, atomistic modelling, and machine learning, we develop predictive frameworks for the design of molecules and materials with targeted functionality. These efforts enable applications in precision agriculture, self-healing infrastructure, and energy storage.

Bio: Dr Francisco Martin-Martinez is a Senior Lecturer in Computational Chemistry and AI at King's College London, where he leads a research group focused on the design of nature-inspired materials using computational chemistry and machine learning. He completed his undergraduate studies in Chemical Engineering at the University of Granada, followed by a PhD in Theoretical and Computational Chemistry. After his doctoral studies, he held a postdoctoral position at the Vrije Universiteit Brussel and subsequently joined the Massachusetts Institute of Technology (MIT) as a Research Scientist, where he worked for nearly six years. In 2020, he was appointed Lecturer in Chemistry at Swansea University, before moving to King's College London in 2024. In 2022, he was recognised as a Google Cloud Research Innovator, collaborating with Google on the development of self-healing infrastructure.



