Project 2.5. Design of highly selective catalysts guided by Artificial Intelligence.

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Unit: Team XI

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Background: The candidate will have the opportunity to carry our world-class research at the intersection of synthetic chemistry, molecular self-assembly, and artificial intelligence to design, synthesize, and characterize unique "hybrid" catalysts allowing for selectively addressing the otherwise chemically equivalent functionalities within organic molecules. The applicant will demonstrate the use of these catalysts in (i) late-stage, site-specific functionalization of medicinally-relevant scaffolds and (ii) in driving novel stereoselective transformations. The applicant will gain solid grounding in synthesis, will learn how to guide molecular design with the tools of artificial intelligence, and will master the instrumental toolkit of modern synthesis. The team the applicant will join is home to some of the Europe's best and brightest young organic chemists (creators of Chematica/Synthia™ – do check it out!) and is led by the Feynman Prize Laureate, Prof. B.A. Grzybowski(https://scholar.google.com/citations?user=hjS0xZ0AAAAJ&hl=en&oi=ao) The applicant will have the opportunity to broaden his/her scientific horizons through close collaboration with world's leading pharma companies and/or short-term visits to Prof. Grzybowski's laboratories in Korea (https://www.ibs.re.kr/softmatt/).

Aim: Have you ever pondered why enzymes are so skillful in catalyzing reactions with such incredible selectivity? Why can enzymes "choose" to perform a reaction on just one of many, apparently equivalent bonds – while man-made catalysts cannot? Could we synthesize in the laboratory, from simple building blocks, catalysts that resemble enzymes in their specificity? Could these "artificial enzymes" be pre-programmed to build themselves up via self-organization? These are precisely the questions our team is asking under Poland's most prestigious Maestro grant. We are combining the tools of organometallic synthesis and supramolecular self-organization to craft precisely such "artificial enzyme" mimics. We do not just re-use amino acids (like enzymes) and we use completely different sets of building blocks to make structures that can function in organic solvents and in elevated temperatures (very much *unlike* enzymes!). We are not "guessing" how these unique constructs should look like, but we guide their design and self-assembly with artificial intelligence, AI. We do not expect you to become an expert in AI but if you join us, you will discover an incredible power of combining synthesis with the tools of AI – it is like synthesis on steroids! At the end of the day, our catalysts promote reactions that have been thought impossible, and modify scaffolds of drug candidates via site-selective late-stage functionalization (this is why we are closely connected with the pharmaceuticals' sector). Altogether, this might all sound like magic, but it is real – if you are intrigued, send us an email and we will be happy to chat!

Requirements: Solid knowledge of chemistry, passion for discovery, and the desire to perform paradigm-shifting research.