Kavli Energy NanoScience Institute (ENSI) (/)

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2023 Graduate Student Fellow

Faculty Advisor: Professor Omar Yaghi

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Zhiling Zheng is currently a 4thyear Chemistry Ph.D. student in the research group of Professor Omar M. Yaghi, working on the synthesis and study of new metal–organic frameworks (MOFs) for atmospheric water harvesting. Before attending UC Berkeley, Zhiling received his B.A. in chemistry and chemical biology from Cornell University. In his free time, he loves traveling, hiking, exploring national parks, and shooting landscapes.

Water is an indispensable component of life, yet water scarcity has been one of the most significant long-term challenges facing society today. To date, several porous MOFs have been identified as candidate sorbents for direct atmospheric water harvesting and, among them, MOF-303 {[Al(OH)(PZDC)], where PZDC2- is 1H-pyrazole-3,5-dicarboxylate} was recently successfully deployed for harvesting moisture from the air. During his fellowship, Zhiling aims to investigate how the multivariate strategy of making nanoscale MOFs provides a handle for controlling the hydrophilic nature of the pores and, consequently, the regeneration temperature and heat, as well as the humidity cut-off at which MOF-303 can operate.

As the working relative humidity (RH) ranges of most single-linker MOFs are narrow, it remains challenging to obtain synthetically tunable MOFs with different humidity cut-off ranges and heat of adsorption energies to be adaptive to complicated real-world conditions. Therefore, it is imperative to develop new approaches to synthesize MOFs based on multivariate linkers, which can be easily tailored to a variety of environmental conditions for efficient atmospheric water harvesting.

Energy Harvesting, Conversion and Production in Nanoscale Natural and Synthetic Systems

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2022 Kavli ENSI Thesis Prize

Please join us in congratulating Nikita Hanikel and Stefano Cestellos Blanco, who were awarded the 2022 Kavli Thesis Prize. The prize is given to the student with the outstanding thesis, publication status, strength of supporting letters and relevance of the thesis to the Kavli ENSI mission. The award provides a $2,000 stipend and an award certificate.

Stefano Cestellos-Blanco
Advisor: Prof. Peidong Yang

Sustainable CO2 valorization by coupling electro- and biocatalysis

Earth's average surface temperature has risen by over 0.84 °C caused by the increase of CO2 in the atmosphere. Renewable energy generation such as solar-to-electricity conversion has been developed over the past few decades. Yet we continue to burn more fossil fuels than ever as these technologies are hampered by intermittency and the difficulty of storing harvested energy. Photosynthesis provides a blueprint for capturing and storing solar energy in chemical bonds. However, our energy demands realistically outstrip its poor solar-to-biomass efficiency and its long timescales. Cestellos-Blanco's thesis focused on developing photosynthetic biohybrid systems which employ light harvesting semiconductor materials paired with CO 2 -consuming bacteria for the solar-driven conversion of CO 2 and N 2 to value- added chemicals and materials. These functional materials provided the "living" biocatalysts with energy which promoted CO 2 fixation with high selectivity and low activation energy. In more detail, Cestellos-Blanco explored the interface between light-active silicon nanowires and bacteria that take up electrons to power the conversion of CO 2 into acetate. Building on this, through co-culturing of different bacterial strains, a complete biomanufacturing platform was realized where acetate served as an upgradeable carbon intermediate to produce printable polymers and fertilizer. Furthermore, engineered material platforms were employed to culture bacterial biofilms for improved access to redox molecules, thus increasing the rate of CO2 fixation. Finally, Cestellos-Blanco demonstrated a novel method to convert CO2 to sugars abiotically by coupling electrocatalysis and prebiotic chemistry. These sugars could be consumed by Escherichia coli - unlocking rapid biomanufacturing of a vast array of chemical products from CO2.

Nikita Hanikel
Advisor: Prof. Omar Yaghi

Atmospheric Water Harvesting with Metal–Organic Frameworks

Advancement of supplemental methods for freshwater generation is imperative to effectively address the global water shortage crisis. In this regard, extraction of the ubiquitous atmospheric moisture is a powerful strategy allowing for decentralized access to potable water. The energy requirements as well as temporal and spatial restrictions of this approach can be substantially reduced if an appropriate sorbent is integrated in the atmospheric water generator. Accordingly, Nikita's thesis focuses on development, characterization, and practical utilization of metal–organic frameworks (MOFs) as sorbents for water capture from air. In particular, the molecule-by-molecule water uptake mechanism in the state-of-the-art water-harvesting MOF is discerned by utilizing single-crystal X-ray diffraction analysis. Equipped with this knowledge, a strategy to deliberately shape the water-harvesting properties through the multivariate approach is developed. This allows for a reduction in desorption temperature and heat, as well as tuning of the operational humidity range without compromises to water uptake capacity and hydrothermal stability. To facilitate the industrial utilization of these materials, a novel, high-yielding synthetic method is devised, which allows for kilogram-scale production of water-harvesting MOFs. Lastly, the water mobility in these materials is probed and the water diffusion mechanism is uncovered. The insights from studying the water uptake kinetics are implemented in a new and highly productive atmospheric water harvester relying on fast uptake and release cycling. The prototype is successfully deployed in the Mojave Desert, thus establishing MOF-assisted water harvesting as a viable strategy to address water scarcity in arid climates.

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