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The hydrogen bond is one of the most versatile units of chemical, material and biological systems facilitating water's many anomalous properties, promoting efficient proton transport in fuel cell membranes, and endowing catalytic functionality in enzymatic reactions. The hydrogen bond arises from the interplay of the quantum mechanical behavior of the light hydrogen nucleus and its electrons. In this talk I will show how our recent developments, which allow us to efficiently simulate the quantum mechanical nature of both the nuclei and electrons, provide insights into how hydrogen bonds are harnessed in chemical and biological processes ranging from the atmospheric separation of hydrogen isotopes, to the spectroscopy and transport of aqueous protons, and proton delocalization in enzyme active sites.

Frances Hamilton Arnold ¹

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Not satisfied with nature's vast catalyst repertoire, we want to create new protein catalysts and expand the space of genetically encoded enzyme functions. I will describe how we can use the most powerful biological design process, evolution, to optimize existing enzymes and invent new ones, thereby circumventing our profound ignorance of how sequence encodes function. Using mechanistic understanding and mimicking nature's evolutionary processes, we can generate whole new enzyme families that catalyze synthetically important reactions not known in biology. Recent successes include selective carbene insertion to form C-Si and C-B bonds, and alkyne cyclopropanation to make highly strained carbocycles, all in living cells. Extending the capabilities and uncovering the mechanisms of these new enzymes derived from natural iron-heme proteins provides a basis for discovering new biocatalysts for increasingly challenging reactions. These new capabilities increase the scope of molecules and materials we can build using synthetic biology and move us closer to a sustainable world where chemical synthesis can be fully programmed in DNA.