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Self-Assembling Uranium Nanostructures

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One of the largest challenges to human progress is the need for continuous, sustainable and clean energy. As the world begins to move away from damaging carbon energy sources such as coal and oil, the need to improve the somewhat controversial nuclear power system becomes evident. Closing the nuclear fuel cycle involves not only cleaner mining techniques but fast, effective environmental remediation and chelation therapy in response to accidental exposure. This project aims to design a uranium ligand technology that can be applied to all three of those areas, with particular interest in mining ocean water where uranium exists as the uranyl dication (UO_2^{2+}) at a natural abundance of 3ppb. The structure of uranium dioxide limits chelation to its equatorial plane, preventing use of traditional metal chelators that coordinate both equatorially and axially. In this project, we design ligand complexes that work with the unusual geometry of UO_2^{2+}. The design process involves selecting likely ligands, and allowing these building blocks to self-assemble around the uranium. The self-assembly process works by using components that can make reversible covalent bonds and self-sort to the lowest energy configuration. In this way, we use the thermodynamics of the system to screen for complexes that are both highly selective and energetically robust. After we find a desirable structure, it can be re-synthesized using a non-dynamic linker and applied to ocean mining or aqueous remediation via attachment to a lattice structure. With over seven billion people on this planet and counting, energy will continue to be at the forefront of our problems. With this research, we hope to help alleviate some of the issues revolving around one of the most prevalent energy production methods.