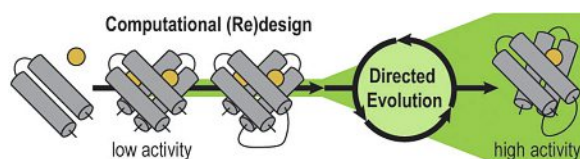


### Evolution of a Highly Active and Enantiospecific Metalloenzyme from Short Peptides

S. Studer, D. A. Hansen, Z. L. Pianowski, P. R. E. Mittl, A. Debon, S. L. Guffy, B. S. Der, B. Kuhlmann, D. Hilvert\*, *Science* **2018**, 362, 1285. ETH Zurich

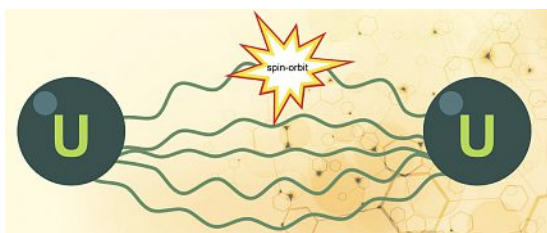
Most metalloenzymes exhibit extraordinarily high catalytic activity and substrate specificity as the result of millions of years of evolution. In their recent publication, Hilvert and coworkers recapitulated a possible mechanism of metalloprotein biogenesis from short peptides. Starting from the homodimeric, zinc-binding MID1-peptide, several rounds of targeted and random mutagenesis were combined with computational redesign to simultaneously re-optimize structure and function. The active site of the generated globular enzyme MID1sc10 esterase strongly resembled that of native zinc enzymes, while exhibiting a high catalytic activity ( $k_{\text{cat}}/K_M \sim 10^6 \text{ M}^{-1} \text{ s}^{-1}$ ) and high enantioselectivity. The novel and innovative approach therefore not only offers insights into the putative biogenesis of these natural catalysts, but also contributes greatly to the scientific fields of enzyme design and engineering.



### Relativistic Quantum Chemical Calculations Show Quadruple Bond in Uranium Molecule $\text{U}_2$

S. Knecht\*, H. J. Jensen, T. Saue, *Nat. Chem.* **2019**, 11, 40. ETH Zurich

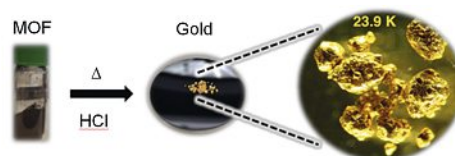
Insight into the bonding of actinides is still limited due to relativistic effects and complicated electronic structures. Stefan Knecht and co-workers have looked deeper into the nature of chemical bonds in the naked diuranium molecule  $\text{U}_2$ . Previous computational studies on this emblematic molecule included only scalar-relativistic effects and neglected spin-orbit interactions; thus, concluding that diuranium has a quintuple bond. In this report, state-of-the-art relativistic quantum chemical calculations suggest the presence of a quadruple rather than quintuple bond for  $\text{U}_2$  along with a change of the nature of the electronic ground state. These new findings support the value of a relativistic multiconfigurational electron correlation approach to predict the electronic structure and molecular properties of bonding interactions between heavy elements.



### Extraction of Gold with a Metal-Organic Framework (MOF)/Polymer Composite

D. T. Sun, N. Gasilova, S. Yang, E. Oveisi, W. L. Queen\*, *J. Am. Chem. Soc.* **2018**, 140, 16697. EPFL.

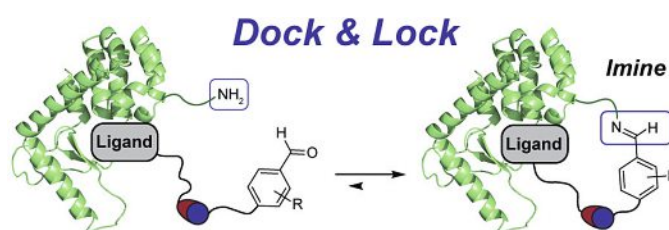
Due to the rise in electronic production, there is an increasing need for electrically conductive and corrosively resistant metals, such as gold. However, mining gold from virgin ore is laborious, costly, and often environmentally unfriendly. This, combined with its limited, diminishing supply, has sparked much interest towards the extraction of gold from a variety of other sources. The Queen group addressed this challenge by developing metal-organic framework (MOF) polymer composites that are capable of extracting trace amounts of gold directly from water sources. In this report, the group demonstrated that the MOF composite is capable of removing >90% of  $\text{Au}^{3+}$  from a variety of real world water sources, including fresh, ocean, and waste water, and solutions used to leach metals from sewage sludge ash and electronic waste. Furthermore, due to the MOFs porosity, it is capable of extracting as much as 934 mg gold/g in a record-breaking rate of less than 2 minutes.



### Affinity Enhancement of Protein Ligands by Reversible Covalent Modifications

A. Dal Corso, M. Catalano, A. Schmid, J. Scheuermann, D. Neri\*, *Angew. Chem. Int. Ed.* **2018**, 57, 17178. ETH Zurich

Protein ligands capable of reversible covalent bonding to amino acid residues are potentially important for the discovery of potent new drugs. Neri and co-workers systematically analyzed the ability of aromatic aldehydes to react with lysine to form imines. Based on these results, they developed a “dock-and-lock” procedure involving complementary LNA strands modified with a protein ligand and 2-hydroxybenzaldehyde. Non-covalent binding between the ligand and protein brought the 2-hydroxybenzaldehyde moiety into close proximity with a lysine residue such that a Schiff base was formed to increase the binding affinity of the complex. This strategy is highly promising for selective *in vivo* modifications of target proteins for potential pharmaceutical and chemical biology applications.



Prepared by Verena Schreier, Aaron Johnson, Ashkan Karimi, Morten O. Loehr, and Nathan W. Luedtke\*

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