Atomic gold mining

The target molecules of the project were the five butanethiols, each with one thiol group and four carbon atoms. Of these R- and S-2-butanethiols are chiral molecules. They are each other’s mirror images, but in fact different molecules.

“The butanethiols display an amazing variety of SAM patterns determined by very subtle surface chemistry and by interactions between the R-groups,” Jingdong Zhang remarks.

Adsorption converts thiols (–SH) to a thiolate (–S–) bound to a gold surface site, Au–S–, which can be a single gold atom or a hollow site between several atoms. This is where the phenomenon "atomic gold mining" comes in. With the exception of one butanethiol, the bulky tertiary butanethiol, which is able to bind directly on a flat surface, the molecules adsorb by digging out surface gold atoms. Hereafter, they bind sideways to the mined gold atom, R-S-Au-S-R.

"The chiral butanethiols open new perspectives. They are the first case for thiol-binding at the same time to mined gold atoms and on the planar surfaces," Jingdong Zhang comments with enthusiasm. "Banding also induces new chiral centres in both the gold surface and the binding sulfur atoms, in addition to the molecular 2-C chiral centre. As a result a "collective" chirality in whole SAM domains arises, leading to the amazing outcome that chiral domains can arise from achiral molecules, and achiral domains from chiral molecules."

The results offer a new level of understanding of the molecular adorption process.

"They will help to understand a wide range of chemical, electrochemical, and spectroscopic phenomena,” according to Jingdong Zhang.

Looking for biofuel catalysis applications

A possible field of application is heterogeneous catalysis in relation to renewable energy, for instance from bio-fuels. Recently, Jingdong Zhang received funding for a project on chemical production of 3D graphene bio catalysts for enzymatic biofuel cells. While the grant is not directly related to the SAM-study published in JACS, Jingdong Zhang hopes to find ways to apply the new nanochemistry findings.

“It is very important for us, as for DTU in general, that fundamental and applied research go hand in hand. Fundamental research is essential to push things to the next level, and applied research is the way we can bring value back to the society which has supported our research. Doing this through applications in clean energy which is highly desirable for society would be really beautiful."

The project on graphene biocatalysts for enzymatic biofuel cells has been granted 0.9 million EUR by the YDUN-program (Younger women Devoted to a University career) of the Danish Council for Independent Research. Besides catalysis, the group’s research on SAMs has potential applications for a number of new synthesis strategies for metallic nanostructures and chemical graphene in chemical and pharmaceutical production and research.