ENGINEERING PROFESSORS DISCOVER FUNDAMENTAL EFFECT IN MONOLAYER CATALYSTS

Posted on September 26, 2017
By: Laurie Fickman

Two professors at the UH Cullen College of Engineering have discovered that size is critical to the performance of the monolayers of catalysts, the fundamental substance that speeds up reactions in all industries from petrochemical to manufacturing. Stanko Brankovic, professor of electrical and computer engineering, and Lars Grabow, professor of chemical and biomolecular engineering, published their findings in the *Journal of American Chemical Society*, one of the most prestigious journals for scientific work in the field of natural sciences.

Capping a two-year project for Brankovic and his Ph.D. student Qiuyi Yuan, their work brings attention to the fundamental effect of finite size in platinum (Pt) catalyst monolayers. “This was ignored in the current understanding of the catalyst monolayers activity,” said Brankovic. He and Yuan measured carbon monoxide absorption in Pt monolayers on Palladium (Pd) single crystal surfaces. What troubled Brankovic were inconsistent findings.

**Launching the team**

It didn’t take long for Brankovic to mention the puzzling phenomenon to Grabow, whose primary research interest is in running complex computer simulations to predict how and why some Pt monolayer catalysts
perform better than others in certain chemical reactions.

?Lars had a hunch that the observed results and monolayer catalyst performance are due to local strain induced by finite size effect,? Brankovic said.

The finite size effect relates to the bonds that form between atoms in a 2D cluster. In a body of atoms, the atoms in the center of the cluster form strong bonds with the surrounding atoms. Atoms located on the periphery of the cluster, however, have asymmetric bonding because there are no atoms on the other side to keep them in equilibrium. This results in the effect that the smaller clusters have more compressive strain and are less active than the bigger ones, inherently making the catalyst monolayer activity size dependent, something the team calls the ?finite size effect.? 

Grabow, along with his graduate student Hieu Doan, ran computer simulations to explain experimental data and identify structures that could obtain favorable catalytic properties due to the finite size effect. Using theoretical calculations to test their hypothesis, Grabow and Doan confirmed that the finite size effect contributed to the catalyst monolayer activities.

?They found that the finite size effect in the Pt/Pd system is huge and has a dominant role in determining its catalytic properties which is the information that can bring much more new development in catalyst monolayer synthesis. ?The morphology of the catalyst monolayer controls their activity,? Brankovic said.

?It turned out that everything Lars and Hieu had calculated matched perfectly with the experimental data. ?We all knew that we are on the verge of some big discovery,? Brankovic said.

Both Brankovic and Grabow are winners of prestigious National Science Foundation CAREER Awards, which partially funded this research. Additional funding came in the form of a University of Houston GEAR Award, which offers seed funding to young researchers looking to get projects inside their laboratory off the ground.