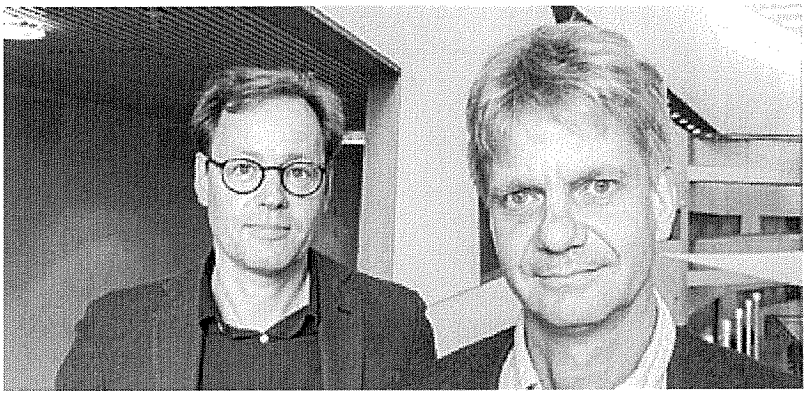
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Grant for catalysis research on atomistic level

(*Nanowerk News*) Professor Magnus Skoglundh from Chemistry and Chemical Engineering has, together with Professor Henrik Grönbeck from Applied Physics, both from Chalmers, been granted SEK 33,530,000 over the course of five years from the Knut and Alice Wallenberg Foundation (KAW) for the project Atomistic Design of Catalysts. They will produce a new research methodology that, on atomistic level, will enable customisation of the next generation of catalysts, which may become the cornerstones of future energy systems.



Magnus Skoglundh and Henrik Grönbeck.

A catalyst is a substance that increases the rate of a chemical reaction, without becoming consumed. The project addresses heterogeneous catalysis, which means that when molecules come in contact with the catalyst's surface, they are affected by the surface's electrons and converted into new molecules. Catalysis both occurs in nature and is used industrially on a large scale. Over 90 percent of all chemicals are produced using catalysts, and they are, for example, needed to produce renewable fuels. New knowledge on catalysts will enable harmful processes to be replaced by environmentally friendly alternatives.

"Catalysis constitutes such a major part of production that development of catalysts is entirely decisive for the future. Without progress, we will not be able to achieve an energy-efficient society," says Magnus Skoglundh.

The research team, which consists of researchers from Chalmers (in addition to Magnus Skoglundh and Henrik Grönbeck also Per-Anders Carlsson and Anders Hellman), Lund University and the Max IV synchrotron facility in Lund, will produce a method that in the future may become the leading way to design catalysts. With funding from the KAW Foundation for the project Atomistic Design of Catalysts, they will, amongst other things, take on the challenging task of creating a short cut in the production of methanol directly from methane. Methanol is currently produced through several catalytic steps, but the new method is expected to be

effective to the extent that methanol could be produced in a single catalytic reaction, which would increase profitability in production and reinforce methanol's position as alternative fuel.

"In the world of catalysis, being able to produce methanol through direct partial oxidation would be something of a dream reaction. In this process, methane becomes methanol by adding oxygen, something which is not yet possible to do industrially," says Magnus Skoglundh.

The primary aim of the project, however, is to develop a new methodology that can be used for several different types of reactions. Direct partial oxidation of methane to methanol is one example of a very difficult key reaction the team hopes to achieve.

In order to succeed with this reaction and many others, researchers are going down to atom level. The surface on which the catalytic reactions take place must be adjusted so that the atoms are optimally placed for the catalytic reaction.

"It is a matter of how the electrons move. We calculate what is happening during the reaction and how the atoms should be arranged to achieve better results. The computational methods have become so powerful that it is now possible to predict how the catalysts will function before the material is even produced. It has not been possible to do this before now. This is one of the most fascinating scientific advances that have been in made in the past twenty years," says Henrik Grönbeck.

The researchers say that primarily two scientific advances have made the current project possible. The technical and theoretical development during recent years has resulted in the possibility to conduct quantum mechanical calculations on how electrons behave when molecules come into contact with different surfaces, at the same time that the thoroughly modern Max IV synchrotron facility will be ready for use. From the point of view of the project, Max IV will make it possible, with synchrotron light, to measure what is happening on atom level in a catalytic reaction, which has not been possible previously.

"We can study a catalytic reaction in the Max IV laboratory and obtain a large amount of data. We then use quantum mechanics and a great deal of computational resources to interpret the data to give it a physical reality and compute what will happen if we modify the structure of the surface," says Magnus Skoglundh.

It is also possible to follow the reaction while it is in progress. Some catalysts are most effective at certain conditions, which will be possible to measure with synchrotron light. It will also be possible to take the optimal conditions into account in the calculations.

"In order to make progress in catalysis research, we have to know what happens when the reaction is happening. This has been very difficult thus far," says Henrik Grönbeck.

The grant from KAW will enable additional new doctoral students to be hired to work on developing the method and explore the different catalytic reactions on a level that has not previously been possible.

"The funding constitutes a substantial contribution to catalysis research at Chalmers and the Competence Centre for Catalysis (KCK). With a grant of this size, we can take large steps forward," says Henrik Grönbeck.

Source: *By Mats Tiborn, Chalmers University of Technology*

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