Green Indicator

With the advent of evermore powerful computer simulation software and hardware, the possibility to perform simulations of advanced reactions and interaction-types are becoming feasible. In this issue of the green indicator, the CatScan section will focus on just this: using quantum mechanics-based calculations for predicting the effects of promoters in catalytic systems. We will also try to plant some thoughts in the area of "what can I do" with respect to helping the environment in our daily life.

/ Christian Hulteberg

What Can We Do

Sometimes people ask me what they can do themselves to help the environment and lower their impact on the earth's resources. This question is treacherous in its simplicity since the question of environment and ecosystems are so complex. Just take the questions of ecologic food and fuel vs. food debate as examples. However, is should be possible to find ways to make small changes to your behavior which has an impact on your resource consumptions.

As I said this is a complex question and many people have put thought into what may be altered behavior wise, one of these are Johan Tell from which I've borrowed much of the tips and tricks. Many of the things that you can do don't really influence your daily life. One such thing is to ensure that you have the correct air-pressure in your tires. With the correct tire pressure you can easily save both fuel and hence reduce your CO_2 emissions; similar effects can be reached just by sticking to the speed limit.

Another tip is to turn of electric appliances and not leave them in stand-by mode. Even laptops, at least older models, that are turned off will consume electricity when trying to load the battery in vain. Using an energy meter is a good way to conclude which cables that can stay connected and which should be disconnected when not used. Another obvious action item is to close all lights in rooms that are not currently used.

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Promoters

There is nothing as elusive or subtle in catalysis as the use of promoters. Adding small amounts, sometimes fractions of a percent, of a compound to a catalyst could radically change the performance of said catalyst; in either direction should be added. Promotion can be performed in many ways and have an impact on several aspects of the catalyst. Such ways include longevity, activity and selectivity by changing both the carrier and the active phase. The addition and discovery of promoters have for many years been dominated by trial and error.

However, in recent years the use of quantum mechanics or molecular mechanics calculations has proven useful in predicting the modus operandi of active sites and the effects of promoters on the sites. In a rather resent paper (Catalysis Today 93 (2004) 535) a group of researchers managed to determine a quantitative model for the synthesis of methanol and also shed light on the electronic structure, properties and stability of promoters on both internal and external surfaces in catalyst supports. Using this type of calculations, it could e.g. be concluded that

Save water. In some places of the world, water is scarce and conserving it is a necessity. However, even in areas without water shortage, the pumping, cleaning and heating of water will consume unnecessary energy. There is however one aspect where water shouldn't be saved and that is when it's used as a beverage. Tap water is the beverage with the best environmental footprint and should be used if possible.

The list can go on and on, but in closing there is one very important thing that I would like to highlight: children. Make them used to spending time in nature, go canoeing, camping, design and build a bird house; make it natural for them that weekends means packing your rucksack and heading out into the forest. Anything, anytime, anywhere, but make sure that the kids learn that nature is worth spending time in and preserving.

surface was unlikely to result in any stabilization of a $Cu/ZnO/Al_2O_3$ catalyst; instead the catalysts should be prepared via metal deposition from aqueous solutions.

This type of calculations will certainly prove to be more and more useful in predicting catalyst behavior, but there are still limitations. The sites considered are all optimal and clearly defined, unfortunately an industrial catalyst is much more inhomogeneous and to fully understand the behavior of a catalyst surface non-ideal sites must be simulated and combined with the ideal ones. It is, as in all theoretical work, important no to lose touch with the experimental side of catalyst design and to use these two elements together for improving the accuracy of the predictions.

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