



Molecular and Nanoscale Catalysts for Hydrogen-Storage (MaNCatal-H2)

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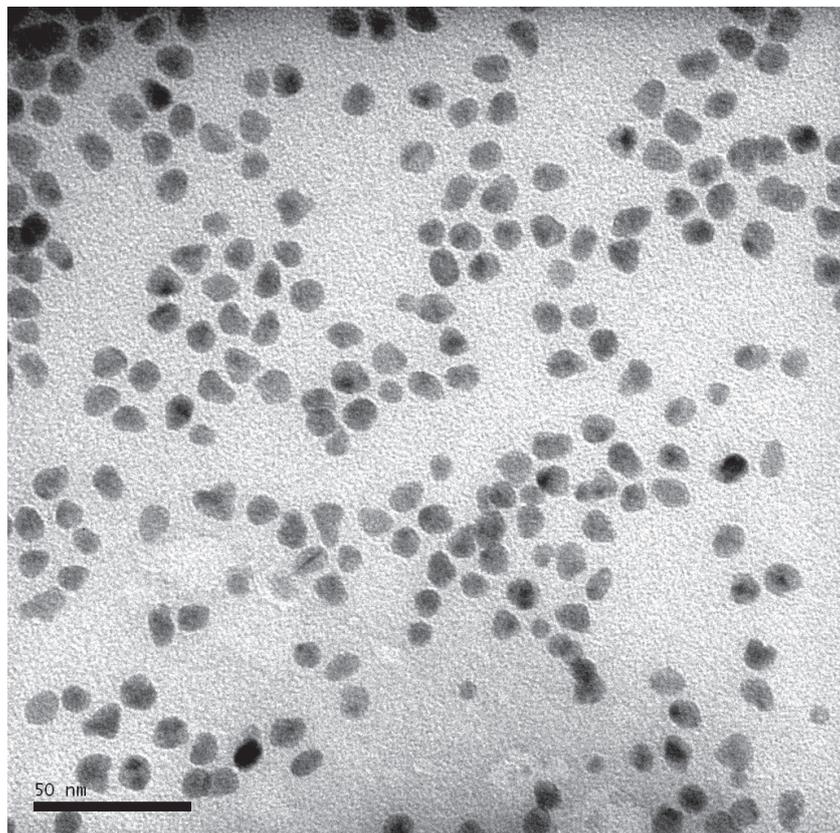


Fig. 1: TEM image of mono-dispersed Pd(0) nanoparticles in IL (scale 50 nm; 500k magnification at 120 kV)



Fig. 2: Mono-dispersed nanoscale metal(0) catalyst (ca 7 nm) immobilized in ionic liquids (IL) in a biphasic system with an organic solvent.

In recent years, an increasing demand for catalytic transformation of renewable raw materials has been recognised. Such raw materials are available in large amounts as energy sources and substrates for the production of bulk and fine chemicals. The investigation of possible renewable energy sources /storage such as vegetable oils, biomass or CO₂ is a great challenge for the scientific community, especially for sustainable technologies. The technical approaches for organic synthesis and energy research involve molecular metal complexes for homogeneous catalysis and nanoscale materials in heterogeneous catalysis for the conver-

sion of biomass. Large amounts of "bio"-alcohols are readily available from renewable sources, such as sugar cane (Brazil), corn (USA, Mexico), cellulose (Canada, Scandinavia, USA) or plant oils for the "bio"-diesel production derived soy bean oil (Brazil), or rape seed oil (Germany). "Bio"-alcohols are used as combustion fuels, producing simply water and CO₂, here "bio"-alcohols are described as CO₂-neutral. However, the agriculture uses fertilisers and agrotocics, which both influence the neutrality of the CO₂-cycle.

Materials

As an innovative alternative for the current use of "bio"-alcohol as combustion fuels, the project MaNCatal-H2 focuses on biomass-based molecules for H₂-storage. Those tailor-made hydrogen storage materials are complement for "bio"-fuels. Attractive molecules for hydrogen storage are for example methanol, ethanol or formic acid. All these molecules have in common a light molecular weight, relatively high hydrogen storage capacity and low costs. Such materials and others can be derived from biomass. Moreover, these materials might be also suitable to reduce the world-wide CO₂ emission by simple use for emission-free H₂-storage and not combustion to CO₂. Furthermore, the efficiency factor of common combustion engines is not higher than 30%, and this can be optimized by H₂-based systems. The drawbacks of current H₂-storage systems are high costs, short life-time, high weight, low capacity, temperature and safety aspects (flammability, explosion hazard, cryogenic techniques).

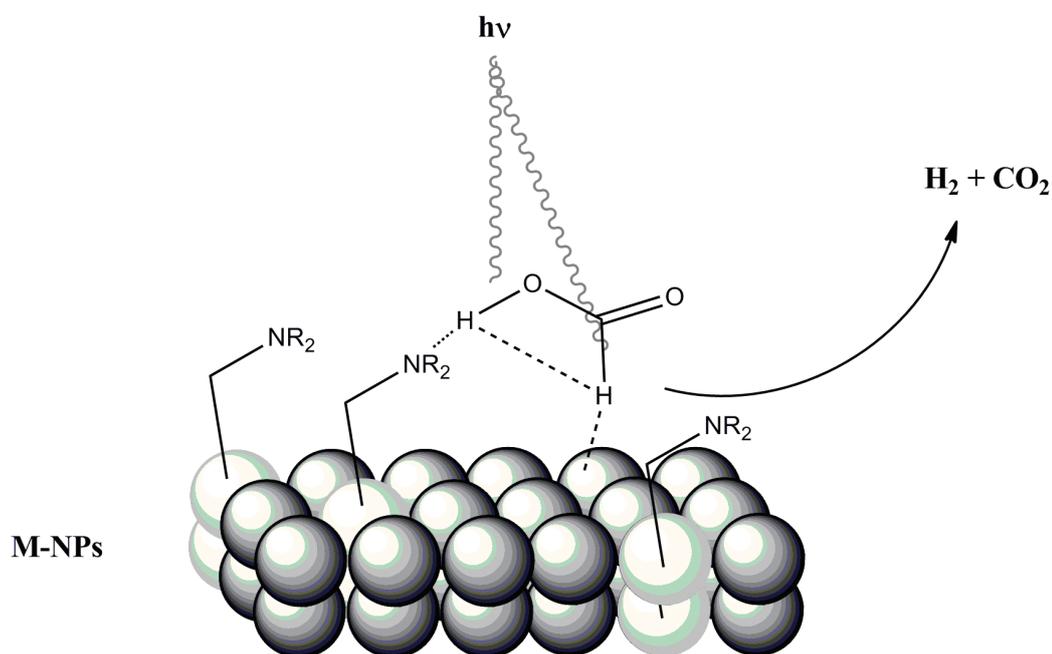


Fig. 3: Nanoscale hybrid catalysts for H₂-generation under visible light.

Catalysis

For more effective H₂-storage we want to develop new nanoscale and molecular metal hydrides catalysts with pincer ligands which are highly active for dehydrogenation (H₂-generation) and hydrogenation (H₂-storage). Moreover, it is important to develop new catalytic systems to close the energy gap with innovative H₂-storage due to the limited fossil sources which is substantial for a more sustainable synthetic chemistry. The chemical and pharmaceutical industry strongly depends on molecular building blocks derived from fossil petroleum. And, this gap of natural resources must be compensated with synthetic building blocks derived from renewable resources through novel technologies.

Outlook

In summary, we develop molecular and nanoscale catalyst systems for sustainable and environmental benign chemistry with a focus on hydrogenation and dehydrogenation processes for H₂-storage and syn-

thetic tools. Especially for the synthesis of novel H₂-storage materials and for further development in the field of activation of small molecules to make them feasible for 21st century H₂-storage materials. As tools for these applications we will develop new cooperative ligands and nanoscale hybrid catalysts. Our studies include mechanistic aspects of catalytic processes for more in-depth understanding to develop tailor-made catalysts. All synthetic aspects focus on the development of sustainable methods with high atom economy and selectivity to avoid waste and by-products.

References

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Martin Prechtel studied chemistry (99-04) in Wuppertal and São Paulo (Brazil). After research at the Max-Planck-Institute for Coal Research, he obtained his Ph.D. from RWTH Aachen in 2007. As Humboldtian he performed research in Porto Alegre (BR) and in Berlin (07-10). He received the Scientist Returnee Award 2009 (MIWF-NRW; W2) and accepted a call to Cologne as independent group leader in 2010. His main interest is catalysis and hydrogen storage.