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From Single Atoms to Bimetallic Clusters and Nanostructured Surfaces: Selective Dehydrogenation & Hydrogen Production

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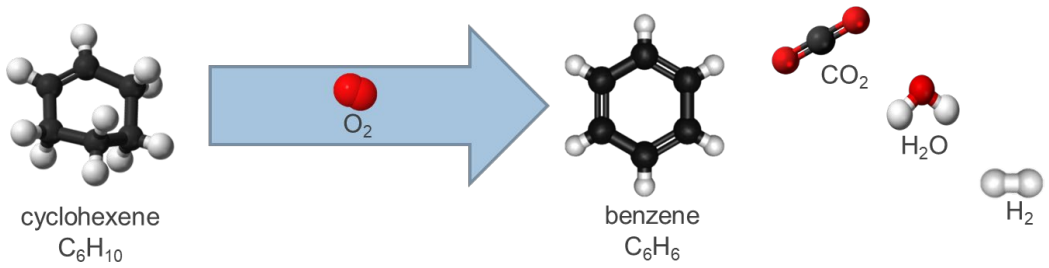
The presentation will, on the example of cyclohexene as model compound, provide an overview of tunability of catalyst performance in function of the size and composition of the catalytic active site and support materials.

The primary focus of the studies is on achieving high selectivity in the oxidative dehydrogenation of cyclohexene to benzene on mono- and bimetallic atomic CuPd clusters of well-defined size and composition[a,b] and single Cu and Pd atoms.[a,b]

In the second part of the presentation, emerging results on the use of atomic clusters towards efficient hydrogen production[c] will be shown, along with the expansion of the materials search place to nanostructured bimetallic films.[c]



From oxidative dehydrogenation to hydrogen production

References:

a) Jašík, J.; Valtera, S.; Vaidulych, M.; Bunian, M.; Lei, Y.; Halder, A.; Tarábková, H.; Jindra, M.; Kavan, L.; Frank, O.; Bartling, S.; Vajda, Š. Oxidative dehydrogenation of cyclohexene on atomically precise subnanometer $Cu_{4-n}Pd_n$ ($0 \leq n \leq 4$) tetramer clusters: The effect of cluster composition and support on performance. *Faraday Discuss.* **2023,** *242*, 70-93. DOI: 10.1039/D2FD00108J, link
b) Valtera, S.; Jašík, J.; Vaidulych, M.; Olszówka, J.E.; Zlámalová, M.; Tarábková, H.; Kavan, L.; Vajda, Š. Atom by Atom Built Subnanometer Copper Cluster Catalyst for the Highly Selective Oxidative Dehydrogenation of Cyclohexene. *J. Chem. Phys.* **2022**, *156*, 114302-114310. DOI: 10.1063/5.0065350, link
c) *in preparation*