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Tuning optical and catalytic properties of ligated noble metal clusters by synergistic role of metallic and organic subunits

Vlasta Bonačić-Koutecký[1,2]
[1]University of Split, Croatia
[2]Humboldt University of Berlin, Germany

Theoretical investigation of the linear and nonlinear optical properties of thiolate-protected low nuclearity noble metal clusters will be first presented. In this context theoretical approaches for reliable description of two-photon absorption spectra will be addressed. Goal is to design species exhibiting strong one-photon and/or two-photon absorption and emission in the UV-VIS spectral range. We will show that the optical properties can be tuned by creating the appropriate interplay between electronic excitations within the cluster core and selected prototype of ligands. Comparison with available experimental results will be discussed. We conclude that such low nuclearity protected noble metal clusters are promising for bio-labelling and imaging as alternatives to the standard fluorescent probes such as quantum dots or organic dyes. Second, we present our study of small coinage metal hydride ligated nanoclusters showing their capability to release the hydrogen. We propose the concept of synergistic role of ligand and substrate in catalysis on example of formic acid. This new catalyst neatly fits into a zeolite which does not perturb reactivity, thus providing a unique example on how “heterogenization” of a homogenous catalyst for the selective catalyzed extrusion of carbon dioxide from formic acid can be achieved, with important application in hydrogen storage and *in situ* generation of H_2. The above results motivated us to investigate the selective decomposition of formic acid driven by highly porous aluminum based metal-organic framework in order to design new materials for the heterogenous catalysis. Thus, we illustrated that unique optical and reactivity properties of ligated noble metal clusters which can be tuned by appropriate interplay between metallic and organic subunits have significant potential for different applications.

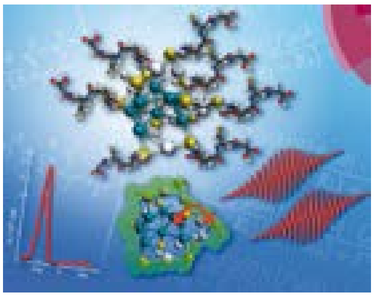

Figure 1: Two-photon absorption of ligand-protected Ag15 nanoclusters. Towards a new class of nonlinear optics nanomaterials

Recent Publications:

1. Z. Sanader, M. Krstic, I. Russier-Antoine, F. Bertorelle, Ph. Dugourd, P. Brevet, R. Antoine, V. Bonacic-Koutecky: "Two-photon absorption of ligand-protected Ag15 nanoclusters. Towards a new class of nonlinear optics nanomaterials.", Phys. Chem. Chem. Phys., 18, 12404 - 12408 (2016.).
2. V. Bonacic-Koutecky: "Theoretical design of new class of optical materials based on small noble metal nanocluster-biomolecule hybrids and its potential for medical applications", Advances in Physics: X, Volume 2, 2017 - Issue 3.
3. I. Russier-Antoine, F. Bertorelle, Z. Sanader, M. Krstic, C. Comby-Zerbino, Ph. Dugourd, P. Brevet, V. Bonacic-Koutecky, R. Antoine: "Ligand-Core NLO-phores: a combined experimental and theoretical approach of the two-photon absorption and two-photon excited emission properties of small ligated silver nanoclusters", Nanoscale, 2017, 9, 1221-1228.

4. A. Zavras, M. Krstic, Ph. Dugourd, V. Bonacic-Koutecky and R. A. J. O'Hair: "Selectivity Eects in Bimetallic Catalysis: Role of the Metal Sites in the Decomposition of Formic Acid into H_2 and CO_2 by the Coinage Metal Binuclear Complexes $[dppmMM'(H)]^+$", ChemCatChem 2017, 9, 1298-1302.
5. M. Krstic, Q. Jin, G. N. Khairallah, R. A. J. O'Hair, V. Bonacic-Koutecky: "How to Translate the $[LCu2(H)]^+$ - Catalysed Selective Decomposition of Formic Acid into H_2 and CO_2 from the Gas Phase into a Zeolite.", ChemCatChem, accepted manuscript, DOI: 10.1002/cctc.201701594, 2018.

Biography

Vlasta Bonačić-Koutecký is a Professor in a Department of Chemistry, Humboldt University, Berlin. Since 2010 she has established the Interdisciplinary Center for Advanced Science and Technology (ICAST) at the University of Split, Croatia and became a head of Center of Excellence STIM in 2014. In the field of nanoscience Vlasta Bonačić-Koutecký has recognized, before others, that metal nanoclusters (with only few atoms) have unique structural, optical and reactivity properties which are combining molecular-like with metallic features. This added a new unexpected dimension to the traditional nanoscience, introducing small metal nanoclusters into material science within the field of nanocatalysis for renewable energy as well as nanooptics and nano-biosensing for medical diagnostics.

vbk@stim.unist.hr

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