

IA ID IE

M. Krstić, 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 H₂ and CO₂ from the Gas Phase into a Zeolite", *ChemCatChem*, 10(5), 1173-1177, DOI: 10.1002/cctc.201701594, (2018).

M. Waszkielewicz, J. Olesiak-Banska, C. Comby-Zerbino, F. Bertorelle, X. Dagany, A. K. Bansal, M. T. Sajjad, I. D. W. Samuel, Z. Sanader, M. Rozycka, M. Wojtas, K. Matczyszyn, V. Bonacic-Koutecky, R. Antoine, A. Ozyhar and M. Samoc: "pH-Induced transformation of ligated Au₂₅ to brighter Au₂₃ nanoclusters", *Nanoscale*, 10(24), 11335-11341, DOI: 10.1039/C8NR00660A, (2018)

V. Bonacic-Koutecky, M. Perić, Z. Sanader: "Why Do Silver Trimers Intercalated in DNA Exhibit Unique Nonlinear Properties That Are Promising for Applications?", *J. Phys. Chem. Lett.*, 9(10), 2584-2589, DOI: 10.1021/acs.jpcllett.8b00819, (2018).

A. Zavras, A. Mravak, M. Bužančić, J. M. White, V. Bonacic-Koutecky, R. A. J. O'Hair: "Structure of the Ligated Ag₆₀ Nanoparticle [Cl@Ag₁₂@Ag₄₈(dppm)₁₂] (where dppm = bis(diphenylphosphino)methane).", *Chinese J. Chem. Phys.*, DOI: 10.1063/1674-0068/cjcp1812285, (2019).

C. Comby-Zerbino, M. Perić, F. Bertorelle, F. Chirot, Ph. Dugourd, V. Bonacic-Koutecky and R. Antoine: "Catenane Structures of Homoleptic Thioglycolic Acid-Protected Gold Nanoclusters Evidenced by Ion Mobility-Mass Spectrometry and DFT Calculations", *Nanomaterials*, 9(3), 457-463, DOI: 10.3390/nan09030457, (2019).

Richard A. J. O'Hair, Antonija Mravak, Marjan Krstić and Vlasta Bonačić-Koutecký: "Models facilitating the design of a new metal-organic framework catalyst for the selective decomposition of formic acid into hydrogen and carbon dioxide.", *ChemCatChem* 11(10) <https://doi.org/10.1002/cctc.201900346>

H. Fakhouri, M. Perić, F. Bertorelle, P. Dugourd, X. Dagany, I. Russier-Antoine, P.-F. Brevet, V. Bonačić-Koutecký and R. Antoine: "Sub-100 nanometer silver doped gold-cysteine supramolecular assemblies with enhanced nonlinear optical properties", *Phys. Chem. Chem. Phys.*, 21(23), 12091-12099, DOI: 10.1039/C9CP00829B (2019)

V. Bonačić-Koutecký and R. Antoine: "Enhances two-photon absorption of ligated silver and gold nanoclusters: theoretical and experimental assessments", *Nanoscale*, 2019, 11, 12436-12448, DOI: 10.1039/C9NR01826C (2019)

Martina Perić, Željka Sanader Maršić, Isabelle Russier-Antoine, Hussein Fakhouri, Franck Bertorelle, Pierre-François Brevet, Xavier le Guével, Rodolphe Antoine and Vlasta Bonačić-Koutecký: "Ligand shell size effects on one- and two-photon excitation fluorescence of zwitterion functionalized gold nanoclusters", *Phys. Chem. Chem. Phys.*, 2019, 21, 23916-23921. DOI:10.1039/C9CP05262C

Howard Z. Ma, Alasdair I. McKay, Antonija Mravak, Michael S. Scholz, Jonathan M. White, a Roger J. Mulder, Evan J. Bieske, Vlasta Bonačić-Koutecký and Richard A. J. O'Hair: "Structural characterization and gas-phase studies of the [Ag₁₀H₈(L)₆]₂⁺ nanocluster dication", DOI: 10.1039/c9nr08321a, *Nanoscale*

A. Humeniuk, M. Bužančić, J. Hoche, J. Cerezo, R. Mitric, F. Santoro and V. Bonačić-Koutecky: "Predicting fluorescence quantum yields for molecules in solution: A critical assessment of the harmonic approximation and the choice of the lineshape function", *J. Chem. Phys.*, 152, 054107, DOI: 10.1063/1.5143212, (2020.)

A. Mravak, M. Krstić, S. M. Lang, T. M. Bernhardt, V. Bonačić-Koutecky: "Intrazeolite CO Methanation by Small Ruthenium Carbonyl Complexes: Translation from Free Clusters into the Cage", *ChemCatChem*, 12, 3857-3862, DOI: 10.1002/cctc.202000716, (2020.)

S. Basu, M. Perić Bakulić, H. Fakhouri, I. Russier-Antoine, C. Moulin, P.-F. Brevet, V. Bonačić-Koutecky and R. Antoine: "Rationale Strategy to Tune the Optical Properties of Gold Catenane Nanoclusters by Doping with Silver Atoms", *J. Phys. Chem. C*, 124 (35), 19368-19374, DOI: 10.1021/acs.jpcc.0c05402, (2020.)

Alexander Humeniuk, Roland Mitrić, and Vlasta Bonacic-Koutecky: Size Dependence of Non-Radiative Decay Rates in J-aggregates, *The Journal of physical chemistry* <https://pubs.acs.org/doi/10.1021/acs.jpca.0c09074>

Franck Bertorelle, Srestha Basu, Hussein Fakhouri, Martina Perić Bakulić, Pierre Mignon, Isabelle Russier-Antoine, Pierre-François Brevet, Sabu Thomas, Nandakumar Kalarikkal and Rodolphe Antoine: "Covalent anchoring of atomically precise glutathione-protected gold nanoclusters on graphene oxide nanosheets", *Nano Express* 1 (2020) 030005 DOI: 10.1088/2632-959X/abbe31

Evan Rizzel Gran, Franck Bertorelle, Hussein Fakhouri, Rodolphe Antoine, Martina Perić Bakulić, Željka Sanader Maršić, Vlasta Bonačić-Koutecký, Manon Blain, Jack Antel, Dusica Maysinger: "Size and ligand effects of gold nanoclusters in alteration of organellar state and translocation of transcription factors in human primary astrocytes", *Nanoscale* 13, no. 5 (2021): 3173-3183, <https://doi.org/10.1039/DoNR06401G>

Ž. Sanader Maršić, D. Maysinger, V. Bonačić-Koutecky: "Insights into Interactions between Interleukin-6 and Dendritic Polyglycerols", *Int. J. Mol. Sci.*, 22 (5), 2415, DOI: 10.3390/ijms22052415, (2021.)

A. Halder, C. Lenardi, J. Timoshenko, A. Mravak, B. Yang, L. K. Kolipaka, C. Piazzoni, S. Seifert, V. Bonacic-Koutecky, A. I. Frenkel, P. Milani and S. Vajda: "CO₂ Methanation on Cu-Cluster Decorated Zirconia Supports with Different Morphology: A Combined Experimental In Situ GIXANES/GISAXS, Ex Situ XPS and Theoretical DFT Study", *ACS Catal.*, 11, 6210-6224, DOI: 10.1021/acscatal.0c0502

S. Daly, S. Weske, A. Mravak, M. Krstić, A. Kulesza, R. Antoine, V. Bonacic-Koutecky, P. Dugourd, K. Koszinowski, R. A. J. O'Hair: "Phenyl argentate aggregates [Ag_nPhn+1] – (n = 2 - 8): models for the self-assembly of atom-precise polynuclear organometallics", *J. Chem. Phys.*, 154, 224301, DOI: 10.1063/5.0052697, (2021.)

Dusica Maysinger, Željka Sanader Maršić, Evan Rizzel Gran, Adeola Shobo, Jun-Ray Macairan, Issan Zhang, Martina Perić Bakulić, Rodolphe Antoine, Gerhard Multhaup, and Vlasta Bonačić-Koutecký: "Insights into the Impact of Gold Nanoclusters Au₁₀SG₁₀ on Human Microglia", *ACS Chemical Neuroscience* 2022 13 (4), 464-476 DOI: 10.1021/acchemneuro.1c00621

Rodolphe Antoine, Dusica Maysinger, Lucie Sancey and Vlasta Bonačić-Koutecký: „Open questions on proteins interacting with nanoclusters“. *Commun Chem* 5, 47 (2022). <https://doi.org/10.1038/s42004-022-00665-9>.

Dr. Franck Bertorelle, Dr. K. David Wegner, Martina Perić Bakulić, Hussein Fakhouri, Clothilde Comby-Zerbino, Dr. Amin Sagar, Dr. Pau Bernadó, Dr. Ute Resch-Genger, Prof. Vlasta Bonačić-Koutecký, Dr. Xavier Le Guével, Dr. Rodolphe Antoine: "Tailoring the NIR-II Photoluminescence of Single Thiolated Au₂₅ Nanoclusters by Selective Binding to Proteins". *Chemistry—A European Journal* 28,39 (2022) <https://doi.org/10.1002/chem.202200570>

A. Mravak, S. Vajda, V. Bonačić-Koutecký: "Mechanism of catalytic CO₂ hydrogenation: to methane and methanol using a bimetallic Cu₃Pd cluster at a zirconia support", *J. Phys. Chem. C*, 126 (43), 18306-18312, (2022.) + Supplement Cover <https://doi.org/10.1021/acs.jpcc.2c04921>

I. ADVANCED TECHNOLOGY AT NANOSCALE_PUBLICATIONS

V. Bonačić-Koutecký, X. L. Guevel, R. Antoine: "Engineering Liganded Gold Nanoclusters as Efficient Theranostic Agents for Cancer Applications" *ChemBioChem* (2022) <https://doi.org/10.1002/cbic.202200524>

M. Bužančić Milosavljević, A. Mravak, M. Perić Bakulić, V. Bonačić-Koutecký: "Model systems for dye-sensitized solar cells: cyanidin-silver nanocluster hybrids at TiO₂ support", *RSC Adv.*, **13**, 6010-6016 <https://doi.org/10.1039/D3RA00165B>

Anna Pniakowska, Krishnadas Kumaranchira Ramankutty, Patryk Obstarczyk, Martina Perić Bakulić, Željka Sanader Maršić, Vlasta Bonačić-Koutecký, Thomas Bürgi, Joanna Olesiak-Bańska: "Gold-Doping Effect on Two-Photon Absorption and Luminescence of Atomically Precise Silver Ligated Nanoclusters" *Angewandte Chemie* 2022 <https://doi.org/10.1002/anie.202209645>

IB

Tobias Hofmann, Tobias Helbig, Frank Schindler, Nora Salgo, Marta Brzezinska, Martin Greiter, Tobias Kiessling, David Wolf, Achim Vollhardt, Anton Kabaši, Ching Hua Lee, Ante Bilušić, Ronny Thomale, and Titus Neupert: "Reciprocal skin effect and its realization in a topoelectrical circuit", *PHYSICAL REVIEW RESEARCH* **2**, 023265 (2020), DOI: 10.1103/PhysRevResearch.2.023265

IC

Željko Penga, Christian Bergbreiter, Frano Barbir, Joachim Scholta: „Numerical and experimental analysis of liquid water distribution in PEM fuel cells“, *Energy Conversion and Management* **189** (2019) 167–183, DOI: 10.1016.2019.03.082

Zeljko Penga, Gojmir Radica, Frano Barbir, Sandro Nizetic: „Coolant induced variable temperature flow field for improved performance of proton exchange membrane fuel cells“, DOI:10.1016.2018.10.237, 2018 Hydrogen Energy Publications LLC

I. Tolj, Ž. Penga, D. Vukičević, F. Barbir: Thermal management of edge-cooled 1 kW portable proton exchange membrane fuel cell stack. *Applied Energy*, Volume **257**, Article 114038, 2020. (Q1 journal IF 8.426), <https://doi.org/10.1016/j.apenergy.2019.114038>

Mišo Jurčević, Željko Penga, Branko Klarin, Sandro Nižetić: „Numerical Analysis and Experimental Validation of Heat Transfer During Solidification of Phase Change Material in a Large Domain“, *Journal of Energy Storage*, Volume **30**, August 2020, 101543, <https://doi.org/10.1016/j.est.2020.101543>

I. Pivac, F. Barbir: „Impact of Shutdown Procedures on Recovery Phenomena of Proton Exchange Membrane Fuel Cells“, *Fuel Cells*, DOI: 10.1002/fuce.201900174

Lei Xing, Yuanxiang Xua, Željko Penga, Qian Xu, Huaneng Su, Weidong Shi, Frano Barbir: „A novel flow field with controllable pressure gradient to enhance mass transport and water removal of PEM fuel cells“, *Transport phenomena and fluid mechanics*, *Aiche Journal* DOI10.1002/aic.16957

I. ADVANCED TECHNOLOGY AT NANOSCALE_PUBLICATIONS

Xing, Lei; Xu, Yuanxiang; Penga, Željko; Xu, Qian; Su, Huaneng; Barbir, Frano; Shi, Weidong; Xuan, Jin: "A segmented fuel cell unit with functionally graded distributions of platinum loading and operating temperature", *Chemical Engineering Journal*, 406 (2021), 126889, 16
[doi:10.1016/j.cej.2020.126889](https://doi.org/10.1016/j.cej.2020.126889)

Ivan Poljak, Paško Županović, Frano Barbir: "Ex situ measurement of charge carrier concentration in Nafon by Hall effect", *Polymer Bulletin*
<https://doi.org/10.1007/s00289-021-03551-x>

Luka Mihanović, Željko Penga, Lei Xing and Viktor Hacker: „Combining Baffles and Secondary Porous Layers for Performance Enhancement of Proton Exchange Membrane Fuel Cells“, *Energies* 2021, 14(12), 3675; <https://doi.org/10.3390/en14123675>

Yulin Wang, Xiaoi Wang, Gaojian Chen, Chao Chen, Xiaodong Wang, Željko Penga, Ziming Yang, Lei Xing: "Reinforcement of proton-exchange membrane fuel cell performance through a novel flow field design with auxiliary channels and a hole array", *American Institute of Chemical Engineers*, 2021, <https://doi.org/10.1002/aic.17461>

Merit Bodner, Željko Penga, Walter Ladreiter, Mathias Heidinger and Viktor Hacker: "Simulation-Assisted Determination of the Start-Up Time of a Polymer Electrolyte Fuel Cell", *Energies* 2021, 14, 7929. <https://doi.org/10.3390/en14237929>

Andraž Kravos, Ambrož Kregar, Željko Penga, Frano Barbir, Tomaž Katrašnik: "Real-time capable transient model of liquid water dynamics in proton exchange membrane Fuel Cells" *Journal of Power Sources* 541 (2022) <https://doi.org/10.1016/j.jpowsour.2022.231598>

Gaojian Chen, Weidong Shi, Jin Xuan, Željko Penga, Qian Xu, Hang Guo, Huaneng Su, Lei Xing: "Improvement of under-the-rib oxygen concentration and water removal in proton exchange membrane fuel cells through three-dimensional metal printed novel flow fields", *AIChE Journal* 2022 <https://doi.org/10.1002/aic.17758>

Domina Cikatić Šanić, Frano Barbir: "Stand-alone micro-trigeneration system coupling electrolyzer, fuel cell, and heat pump with renewables" *International Journal of Hydrogen Energy* Volume 47, Issue 82, 30 September 2022 <https://doi.org/10.1016/j.ijhydene.2022.08.090>

Jakov Šimunović, Ivan Pivac, Frano Barbir: "Techno-economic assessment of hydrogen refueling station: A case study in Croatia", *International Journal of Hydrogen Energy* Volume 47, Issue 57, 5 July 2022 <https://doi.org/10.1016/j.ijhydene.2022.05.278>

Li Guan, Prabhuraj Balakrishnan, Huiyuan Liu, Weiqi Zhang, Yilin Deng, Huaneng Su, Lei Xing, Željko Penga and Qian Xu: "A Tortuosity Engineered Dual-Microporous Layer Electrode Including Graphene Aerogel Enabling Largely Improved Direct Methanol Fuel Cell Performance with High-Concentration Fuel", *Energies* 2022, 15(24), 9388; <https://doi.org/10.3390/en15249388>

Anita Bašić, Željko Penga, Jure Penga, Nenad Kuzmanić and Sandra Svilović: "Zeolite NaX Mass and Propeller Agitator Speed Impact on Copper Ions Sorption", *Processes* 2023, 11(1), 264; <https://doi.org/10.3390/pr11010264>

Andrej Zvonimir Tomić, Ivan Pivac, Frano Barbir: "A review of testing procedures for proton exchange membrane electrolyzer degradation", *Journal of Power Sources*, Volume 557, 15 February 2023, 232569 <https://doi.org/10.1016/j.jpowsour.2022.232569>

Ivan Pivac, Anamarija Stoilova Pavasović, Frano Barbir: "Recent advances and perspectives in diagnostics and degradation of electrochemical hydrogen compressors", *International Journal of Hydrogen Energy*, Available online 11 February 2023, <https://doi.org/10.1016/j.ijhydene.2023.01.281>

IF

Guillaume F. Combes, François-Xavier Pella, Miroslav Radman: "Cause commune et mécanisme commun aux maladies du vieillissement ?", HAL Id: hal-03049547 <https://hal.archives-ouvertes.fr/hal-03049547> DOI : 10.1051/medsci/2020221

Stéphanie Miserey-Lenkei, Katarina Trajkovic, Juan Martín D'Ambrosio, Amanda J Patel, Alenka Čopić, Pallavi Mathur, Kristine Schauer, Bruno Goud, Véronique Albanèse, Romain Gautier, Melody Subra, David Kovacs, Héléne Barelli and Bruno Antony: „A comprehensive library of fluorescent constructs of SARS-CoV-2 proteins and their initial characterisation in different cell types", *Biol. Cell* (2021) 0, 1–18 DOI: 10.1111/boc.202000158

G. F. Combes, H. Fakhouri, C. Moulin, M. Girod, F. Bertorelle, S. Basu, R. Ladouce, M. Perić Bakulić, Z. Sanader Maršić, I. Russier-Antoine, P-F. Brevet, P. Dugourd, A. Krisko, K. Trajkovic, M. Radman, V. Bonacic-Koutecky and Rodolphe Antoine: " Functionalized Au₁₅ nanoclusters as luminescent probes for protein carbonylation detection", *Commun. Chem.*, 4, 69, (2021.) <https://doi.org/10.1038/s42004-021-00497-z>

Guillaume F. Combes, Ana-Marija Vučković, Martina Perić Bakulić, Rodolphe Antoine, Vlasta Bonačić-Koutecky and Katarina Trajković: "Nanotechnology in Tumor Biomarker Detection: The Potential of Liganded Nanoclusters as Nonlinear Optical Contrast Agents for Molecular Diagnostics of Cancer", *Cancers* 2021, 13, 4206., <https://doi.org/10.3390/cancers13164206>

IG

Viktorija Radotić, Dries Braeken, Petar Drviš, Marta Mattotti & Damir Kovačić: "Advantageous environment of micro-patterned, high-density complementary metal–oxide–semiconductor electrode array for spiral ganglion neurons cultured in vitro", *Scientific Reports* volume 8, Article number: 7446 (2018), DOI:10.1038/s41598-018-25814-w