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ALFRED WERNER FUND, MASTER'S STUDENT SCHOLARSHIPS

The Alfred Werner Fund of the SCS Foundation was established in 2014 and continues the initiatives and projects of the former foundation 'Stiftung für Stipendien auf dem Gebiete der Chemie', also known as the 'Werner Stiftung'. The SCS Foundation is very proud to provide this program in collaboration with the Swiss chemical and pharmaceutical industry.

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Alfred Werner Master's Student Scholarships

The program invites scholarship applications to carry out Master degree studies in Chemistry or Biochemistry at a Swiss University or Federal Institute of Technology.

The Foundation offers 8 to 10 scholarships of CHF 25'000 each as a one-time contribution to the cost of the Master study program. This opportunity targets students from foreign countries in the top 10% of their undergraduate programs. The goal of the program is to bring in young talents to Swiss Universities or FIT or to keep them after the BSc studies in Switzerland.

Partner Universities / Federal Institutes of Technology

EPFL ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE
ETH Eidgenössische Technische Hochschule Zürich Swiss Federal Institute of Technology Zurich
UNI BASEL
u^b UNIVERSITÄT BERN
UNI FR UNIVERSITÉ DE FRIBOURG UNIVERSITÄT FREIBURG
UNIVERSITÉ DE GENÈVE
University of Zurich^{UZH}

The program is supported by

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Winners of the Scholarships 2015–17

We are proud and happy to announce the winners of the Werner Scholarships 2015–17 and wish them all the best for their studies in Switzerland.

- EPFL: Ms ***Cassandra Oji-Okora Ogadimma*** (RU), BSc in chemical engineering and biotechnology, Lomonosov Moscow State University of fine chemical technologies, Russia
- ETHZ: Mr ***Loren Ban*** (HR), BSc in chemistry, Department of Chemistry, University of Zagreb, Croatia
- ETHZ: Mr. ***Riccardo Tarchini*** (IT), BSc in chemical engineering, Departimento di Scienza Applicata e Tecnologia, Politecnico di Torino, Italy
- UniGE: Ms ***Sarah Folliet*** (FR), BSc in chemistry, Department of Organic Chemistry, University of Geneva, Switzerland
- UniGE: Mr. ***Lluc Farrera*** (ES), BSc in chemistry, Facultat De Química, University of Barcelona, Spain
- UniGE: Ms ***Yuting Feng*** (CN), BSc in biochemistry, Department of Chemistry, McGill University, Montréal, QC, Canada
- UniZH: Mr ***Ali Tuna*** (TR), BSc in chemistry, Department of Biomedical Engineering, Istanbul University, Turkey

Winners of the Scholarships 2013–15

Two year ago the following four students received one of the Werner Scholarships and they all successfully finished the Master studies.

- UniGE: Ms ***Ani Baghdasaryan*** (AM), BSc at Yerevan State University, Armenia
- EPFL: Ms ***Amina Saleh*** (EG), BSc at American University in Cairo (AUC), Egypt
- UniZH: Ms ***Jelena Habjanič*** (HR), BSc at University of Zagreb, Croatia
- EPFL: Mr ***Aleksandar Salim*** (CS), BSc at University of Belgrade, Serbia

Summaries of the Master Theses

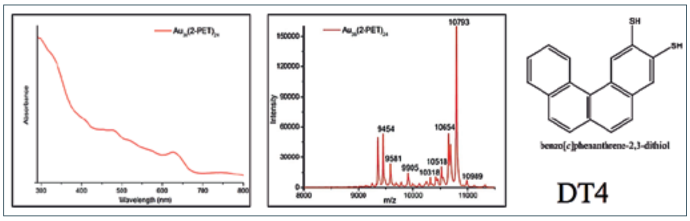
«Ligand exchange reactions on Au$_{38}$: selective arrangements of helical dithiolates»

Ani Baghdasaryan
Nationality: *Armenia*
Bachelor at
Yerevan State University
Master at
University of Geneva
Master thesis supervisor:
Prof. Thomas Bürgi

The aim of this work was the analysis of the ligand exchange of a chiral but configurationally labile dithiolate ligand on chiral Au$_{38}$(2-PET)$_{24}$ cluster in order to elucidate whether the attachment to the chiral cluster stabilizes one enantiomer of the ligand.

*Rac*emic and enantiopure Au$_{38}$(2-PET)$_{24}$ clusters and DT4 ligand were used for exchange reaction.

SEC, HPLC, TLC separation techniques were employed for obtaining pure samples. The products were analyzed using UV-vis and CD spectroscopy and MALDI-TOF mass spectrometry.

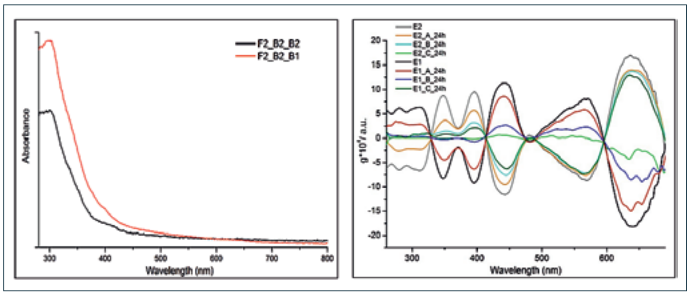


Au_{38}(2-PET)$_{24}$ + DT4; 1:50 ratio

Ligand exchange reaction was run at 50 °C for 48 h.

TLC separation:

1. Band 1- Au_{38}(2-PET)$_{22}$(DT4) one-exchange (10808 Da)
2. Band 2- Au_{38}(2-PET)$_{23}$(DT4) monodentate bonded (10935 Da) products
3. UV-vis features disappear.



CD measurements of enantiopure samples

The mirror image signals at lower wavelengths become smoother and helical properties disappear.

Preparation of Au_{38}(2-PET)$_{24}$

Rac. Au_{38}(2-PET)$_{24}$ educts were prepared according to previously reported protocols.[1,2] The UV-vis spectrum of clusters shows characteristic features at 480, 525 and 600-670 nm. The peak at 10793 Da in the mass spectrum belongs to the cluster.

Conclusions

- Ligand exchange reaction between Au_{38}(2-PET)$_{24}$, enantiopure clusters and DT4 ligand leads to the formation of Au_{38}(2-PET)$_{22}$(DT4) and Au_{38}(2-PET)$_{23}$(DT4)
- UV-vis features at higher wavelengths disappear due to the distortion of the cluster structure;
- TLC method was successfully used for the separation of Au_{38}(2-PET)$_{24-x}$(DT4)$_x$ species;
- The introduction of ligand induces changes of the surface structure and promotes racemization.

[1] S. Knoppe, A. C. Dharmaratne, E. Schreiner, A. Dass, T. Bürgi, *J. Am. Chem. Soc.* **2010**, *132*, 16783.
[2] S. Knoppe, J. Boudon, I. Dolamic, A. Dass, T. Bürgi, *Anal. Chem.* **2011**, *83*, 5056.

Future plans

The obtained results were quite promising and encouraged us to improve the separation procedure. Moreover, the ligand exchange reaction with other chiral thiolate ligands will make an original contribution to the understanding of chiroptical properties of atomically precise gold nanoclusters.

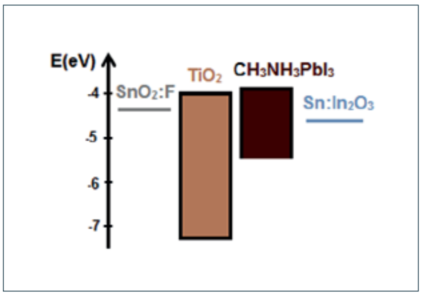
«A fully printable mesoscopic scaffold with Indium Tin Oxide for hole-transporter-free semi-transparent perovskite solar cells »

Amina Saleh
Nationality: *Egypt*
Bachelor at
American University in Cairo (AUC)
Master at
École Polytechnique Fédérale
de Lausanne (EPFL)
Master thesis supervisor:
Prof. Michael Grätzel

Perovskite solar cells are the most recently developed type of solar cells which have caught a lot of attention by scientists because of their promising photovoltaic performance that, in only a few years, surpassed all the alternative technologies based on solution-processed materials.[1] Perovskites have the advantages of large absorption coefficient, high carrier mobility, direct band gap, as well as being formed from Earth-abundant materials.[2]

However, a typical perovskite solar cell incorporates a hole transporting material (HTM) and gold, which are too expensive for scaling up. There are perovskite solar cells which are HTM-free but they cannot be used in tandem geometry, an architecture that combines different cells to boost the overall performance of the device. No HTM-free perovskite cells were reported to be semi-transparent in the infrared (IR) region of the spectrum, the condition required for their participation in tandem cells.

This work presents an HTM-free perovskite cell that could potentially be semi-transparent in the IR (for tandem cells) and/or in the visible region (for windows fabrication). Another advantage of the scaffold is its simplicity: a fully printable mesoporous structure consisting of a TiO_2 layer (for electrons' injection), a tin-doped indium oxide (ITO) layer (for holes' injection), and a layer of Al_2O_3 between them (to prevent recombination). No HTM or gold is needed. To push the accessibility of industrial scale-up further, infiltrating the perovskite solution with the inkjet printing technology was attempted.



The effect of varying the thickness of each of the layers on the photovoltaic performance was studied, as well as that of varying the concentration and the halide composition of the perovskite. A particular attention was given to understanding and decreasing the series resistance of the device. Fundamental characterizations such as measuring the optical properties of the scaffold (with and without perovskite) and the conductivity properties of the ITO were conducted.

[1] Editorial, *Nat. Mater.* **2014**, *13*, 837.
[2] A. Mei, X. Li, L. Liu, Z. Ku, T. Liu, Y. Rong, M. Xu, M. Hu, J. Chen, Y. Yang, M. Grätzel, H. Han, *Science* **2014**, *345*, 295.

«Towards the understanding of unique histidine-rich metallothioneins – protein production, characterization, and investigation of metal ion binding properties»

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Bachelor at
University of Zagreb
Master at
University of Zürich
Master thesis supervisor:
PD Dr. Eva Freisinger

Metallothioneins (MTs) are a superfamily of cysteine-rich proteins with low molecular weight found in all phyla. The precise function of MTs is still a matter of debate, but it is assumed that they have a role in metal homeostasis, provide protection against metal toxicity, and have redox capabilities, hence can act against oxidative stress. The most widely studied MTs are the mammalian forms, and multiple three-dimensional structures are known. From bacteria, only the structure of the SmtA MT from *Synechococcus elongatus* has been explored. The structure of SmtA is unique as it shows several unexpected features for MTs that are absent in the mammalian forms such as a high percentage of secondary structural elements and the presence of aromatic amino acid residues. Most importantly, the structure of SmtA revealed for the first time that also histidine residues can act as metal ligands in MTs.[1]

In my thesis I focused on novel MT sequences from the ubiquitous gram negative bacteria *Pseudomonas fluorescens*, which were shown to contain an unusually high number of histidine residues. These sequences can be divided into three groups distinctive by the length of the sequence, overall charge of the respective protein, and number of His residues. One representative of each group was successfully cloned, over-expressed, purified, and characterized. The investigation of the metal binding abilities of these novel MTs showed surprisingly different metal ion binding properties and mainly lower affinities to Zn^{II} than to Cd^{II}. Surprisingly, the latter finding is in contrast to the properties of SmtA despite the conserved Cys distribution pattern of all four proteins. The three *P. fluorescence* MTs can all bind up to four Cd^{II} ions, but the fourth metal ion is bound less tightly and easily released. Zn^{II} binding is highly dependent on the conditions but mass spectrometry reveals predominantly Zn$_3$ species.

The investigation of spectroscopic features of the novel MTs revealed several interesting, unexpected features previously not observed for MTs, the basis of which has to be further investigated. In addition, the influence of a long C-terminal Cys-free tail in one of the proteins with respect to the metal ion binding abilities was studied and showed no major effect. However, its influence on the binding kinetics and thermodynamic stability cannot be excluded and additional studies are necessary.

Preliminary NMR studies for the determination of the overall 3D structure showed promising results for two of the proteins in their Cd^{II}-bound form, but also here further efforts are needed to arrive at a final structure.

[1] C. A. Blindauer, M. D. Harrison, J. A. Parkinson, A. K. Robinson, J. S. Caavet, N. J. Robinson, P. J. Sadler, *PNAS* **2001**, *98*, 9593.

Future plans

After finishing my master degree I have decided to immediately continue my education on the PhD level. I got a great opportunity to continue working on the project I started during my master program in the group of PD Dr. Eva Freisinger at University of Zurich and I am looking forward to study these exciting new proteins on a deeper level.

«Contributions to Pd(0)-catalyzed C$_{sp2}$–H bond functionalization»

Aleksandar Salim
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Bachelor at
University of Belgrade
Master at *EPFL*
Master thesis supervisor:
Prof. Nicolai Cramer

Recently, there has been extensive research in palladium-catalyzed C–H functionalization reactions. The aim of this work was the investigation of enantioselective Pd(0)-catalyzed C$_{sp2}$-H alkylation as a potential access to desired molecules. The work was performed in the Cramer group. The results will be published in due time.

Future plans

After graduation, I decided to stay at EPFL. I am currently doing a PhD in group of Prof. Kai Johnsson, working on the multidisciplinary project which aims to develop new fluorescent probes for live cell labeling of centrosome. After my PhD my plans are to pursue a career in science and further develop my scientific skills.