Report for Advisory Board of Charles University Centre of Advanced Materials

for time period Aug 2016 - Sep 2018

"CHARLES UNIVERSITY CENTRE OF ADVANCED MATERIALS: DESIGN, SYNTHESIS, AND APPLICATIONS (CUCAM)", OP VVV "Excellent Research Teams", project No. CZ.02.1.01/0.0/0.0/15_003/0000417

Centre Goal: To develop a world-leading Centre of Excellence in Advanced Materials located at Charles University (CU) in Prague, specialising in the Design, Synthesis and Application. The scientific focus of the Centre is on the use of modular (*i.e.* low dimensional) building units for the preparation of new advanced materials, with a particular emphasis on the preparation of hybrid solids. The major vision of the Centre will be to overturn the conventional thinking and practice in materials science by developing methodologies that can target 'unfeasible' materials – that is, materials which cannot be prepared by traditional methods. The importance of such new methodologies is that they will open up routes to materials that have different properties (both chemical and topological) to those we currently have, which in turn opens up new avenues for exploitation.

1. Budget

So far we were able to follow the plan relatively closely, we only had to postpone payment for HRTEM (see below).

(In mCZK)	Total	Invest.	Personal	Consum.	Travel	Overhead
Plan 2016-22	215.2	98.6	77.2	11.5	8.2	19.7
Spending Aug 16 - Sep 18	65.4	34.3	23.0	2.9	1.0	4.2

2. Infrastructure

2.1. Constructions

Following the plan we completely reconstructed

- Synthesis lab
- Catalyst characterization lab
- HRTEM lab

Using other resources, CUCAM now have additional new labs:

- Soft matter lab
- Catalysis lab
- New office space

2.2. Equipment

New equipment installed in CUCAM lab is listed in the Table 2 below (it only includes investments over 1 mil CZK.

Equipment	Cost (in mCZK)
XRD system	7.0
Raman spectrometer	6.5
FTIR	4.0
Adsorption apparatus	5.6
GC-MS	3.6
Autoclave	1.8
Computing server	4.4

In addition, we have ordered new HRTEM JEOL NEOARM that will be delivered in Nov 2018.

HRTEM	44.8
Automatic temperature stabilization system for HRTEM	4.2

3. Personal

Team is stabilized: 16 research position (7 foreigners + 9 Czechs), 1 technician and 3 administrative positions.

In 2019 we only plan 1-2 changes on postdoc positions (depending on the grant application success and individuals performance). We will reduce administrative positions by one since Jan 2019 (public procurement position).

4. Research

The Centre is organized to focus on three major themes:

1. catalytic materials
2. advanced electronic and optical materials
3. next generation functional solids for applications such as medical devices

We reported a total of 62 papers as an output of the Center during first 25 months of the project. Majority of results were reported in journals with IF>3 (the full list of publications is in attachment) and substantial number of publications appear in very prestige journals, including Nat. Chem. (1x), Adv. Mater. (3x), ACS Appl. Mat. Int. (2x), Angew. Chem. Int. Ed. (1x), J. Mater. Chem. (4x), Chem. Mater. (1x), Nanoscale (2x), etc. Below we only report top 5 results (in our judgment) achieved so far, with brief description. More details on the results achieved in the Center up to now will be reported during the AB meeting on Thursday Oct 25th afternoon.

Five most important results of the Center:

1. Mechanism of ADOR process	**Nat. Chem. 9 (2017) 1012-1018**
The Assembly-Disassembly-Organisation-Reassembly (ADOR) mechanism is a new method of preparing inorganic framework materials and, in particular, new zeolites. Using the ADOR approach we can prepare isoreticular families of zeolites with unprecedented continuous control over porosity, and develop designed routes to new materials that would previously have been difficult, or even impossible, to synthesise using traditional hydrothermal techniques. The process is extremely flexible, and starting from the parent zeolite with the UTL framework topology one can prepare a family of six new zeolites, named IPC-2, IPC-4, IPC-6, IPC-7, IPC-9 and IPC-10. Such diversity of outcomes points to a complex mechanism that must be understood if the full potential of the process is to be realised. Here, we report a combination of in situ solid-state nuclear magnetic resonance (NMR) spectroscopy and powder X-ray diffraction (PXRD) experiments that reveal important information about the disassembly, organisation and reassembly steps of the ADOR process. In particular, we use the detailed information on the mechanism to explain the formation of the intriguing structure of zeolite IPC-6.	

2. ADOR - proof of concept	**Angew. Chem. Int. Ed. 56 (2017) 4324-4327**
Assembly-disassembly-organization-reassembly (ADOR) has been demonstrated on UTL parent zeolite in 2013 and so far 12 new zeolite frameworks were obtained by this novel synthesis protocol. This manuscript demonstrates that ADOR is not limited to single parent zeolite (UTL) and that it can be successfully used for (suitable) parent zeolite framework. A novel zeolite framework IPC-12 has been obtained by ADOR from parent UOV zeolite. The structure of the material has previously been predicted computationally and confirmed in our experiments using X-ray diffraction and atomic resolution STEM-HAADF electron microscopy. This is the first successful application of the ADOR process to a material with porous layers.	

3. **Antibacterial Nitric Oxide- and Singlet Oxygen-Releasing Nanoparticles Responsive to Light and Temperature Triggers**	**Nanoscale 10 (2018) 2639-2648**
Herein, we report the preparation, characterization and antibacterial evaluation of sulfonated polystyrene nanoparticles simultaneously releasing two antibacterial species, nitric oxide and singlet oxygen upon irradiation with visible light. The nanoparticles were prepared by simple and scalable processes from nanofiber membranes with an encapsulated NO photodonor and/or ionically entangled tetracationic porphyrin/ phthalocyanine photosensitizers. The release of both species from the polystyrene nanoparticles is controlled by light wavelength and dose, as well as by temperature, which influences the diffusion coefficient and solubility in the polystyrene matrix.Due to the efficient photogeneration of both species at physiological temperature and resultant strong antibacterial action observed on *Escherichia coli*, the nanoparticles are a promising material for antibacterial applications triggered/modulated by light and temperature.	

4. **Triazine-Based Photcatalyst Films**	**Adv. Mater. (2017) 1703399(1-9)**
Mixed-dimensional (2D/3D) metal-free van der Waals (vdW) heterostructures based on triazine (C3N3) linkers were grown on copper surfaces from solution. The material consists of a crystalline 2D phase that is fully sp2 hybridized and provides structural stability, and an amorphous, porous phase with mixed sp2–sp hybridization. Interestingly, this 2D/3D vdW heterostructure grows in a twinned mechanism from a one-pot reaction mixture: unprecedented for metal-free frameworks and a direct consequence of on-catalyst synthesis. Thanks to the efficient type I heterojunction, electron transfer processes are fundamentally improved and hence, the material is capable of metal-free, light-induced hydrogen evolution from water without the need for a noble metal cocatalyst (34 μmol h−1 g−1 without Pt). The results highlight that twinned growth mechanisms are observed in the realm of "wet" chemistry, and that they can be used to fabricate otherwise challenging 2D/3D vdW heterostructures with composite properties.	

5. **New catalytic materials for an energy and chemistry transition**	**Chem. Soc. Rev. themed issue (guest editing)**
A themed issue of Chem. Soc. Rev. has been guest edited by two CUCAM team members. Although there are many reviews on catalysis, the goal of this themed issue was to bring together the most recognized researchers in this field to address from their different perspectives and specific fields the common questions: where we are and which possible step changes towards the future of catalysis have to be taken. The issue covers some of the important aspects of the recent development of heterogeneous catalysis, highlighting critical challenges in the synthesis of different types of catalysts, their detailed characterization, theoretical description of properties of catalysts, and last but not least the real word of catalytic transformations and how to move forward. Following two contributions within this special issue were co-authored by CUCAM team members: "**From 3D to 2D zeolite catalytic materials**" and "**From descriptive computational models to in silico design in heterogeneous catalysis**".	

5. Grant applications

The idea of OP VVV projects is to help to establish the center of excellence. Project team members, and the Center itself, must apply for additional grants. CUCAM team members have obtained several GA ČR projects during last two years. In addition, we have obtained BTHA project („Entwicklung von Designprinzipien für strukturierte Materialien: Synthese, Charakterisierung und Anwendungen“, Bayerisch-Tschechischer Forschungsverbünde, 2017-2020, co-investigator, PI – Prof. Martin Hartmann, Erlangen Catalysis Resource Center), collaborative project with US Army, and exploratory research funded by Solvey.
In 2018 we have applied for number of additional projects including, GA ČR EXPRO, standard GAČR, Czech-Japan CONCERT. Currently we are finalizing application for H2020 Twinning (together with University of St Andrews, Katholieke Universiteit Leuven and Università degli Studi di Milano Bicocca).

6. Risks

OP VVV “Excellent Research Teams” project must report number of deliverables. Among those we identify following two as potentially risky:

- Submit two patents: The systems at Charles University are not well developed for IP protection, and some thought will be required as to how this will be done. We have inventions from CUCAM that are protectable.
- Obtained two H2020 projects

While other deliverables do not require special attention, deliverables given above represent some risk, in particular the last one.