



MIRAI Scientific Session,  
13-14 November 2019,  
Stockholm, Sweden

## Materials Science for Sustainable Development

MIRAI Scientific Session, 13-14 Nov 2019, Stockholm, Sweden

### SCIENTIFIC SESSION AIMS AND GOALS

The importance of bilateral collaboration in achieving scientific goals has been emphasized several times by Swedish and Japanese funding agencies. The agencies committed to strengthen the collaboration already at the MIRAI Seminar 2018 in Tokyo. The workshop in Linköping in May 2019 was an inventory and training session for researchers to prepare a joint application. The November MIRAI Scientific Session in Stockholm will continue with this focus.

This scientific session also continues with the SDG (Sustainable Development Goals) focus which was introduced in Linköping. We will focus on the UN Goal 6: *"Ensure availability and sustainable management of water and sanitation for all"* and the UN Goal 7: *"Ensure access to affordable, reliable, sustainable and modern energy for all"*.

The goal of the scientific session will be to identify grand scientific challenges related to the SDGs. We seek to solve challenges that require cooperative research and competences spanning multiple research areas. The participating researchers will develop a draft of joint research proposal targeting these challenges. There will be an opportunity to discuss, formulate research questions, and learn how to formulate a proposal with high chances of winning the funding. The scientific session will focus on the following research areas:

- Materials for energy devices
- Advanced characterization of materials
- Low dimensional materials and surfaces
- Bio-and bioinspired materials

We will host Professor Anders Nilsson of Stockholm University as the Swedish keynote speaker and Professor Takashi Hayashita of Sophia University, Tokyo, as the Japanese keynote speaker.

The goal of this scientific session is to help researchers understanding how to think about research from a user perspective and how to present complex research problems in a compelling way. We will start off with seminars by two keynote speakers presenting how collaborations



enable solving difficult fundamental science challenges related to the SDGs. After these presentations, new members will introduce their research with short 3-min pitches. Then, the participants will form Swedish-Japanese teams to work in groups. The goal of each group will be to prepare an outline of joint proposals targeting the grand challenges of their research fields.

During the parallel session on Wednesday (10:30-15:30, before the NABC session), the participants will work in small groups, and within these groups identify concrete scientific challenges that if solved would advance the research field. Methods and techniques required to solve these problems shall be discussed as well.

The parallel session on Wednesday will finish with 5-min pitches where the groups will present these challenges and their joint approach to solve them. There will be 2-3 minutes after each pitch for other participants to question the problem and the solution method. The pitches must address the following questions:

- Who is the group of researchers?
- Why is this research important?
- What is the research gap today?
- Why this problem needs to be solved?
- What will be a long-term benefit for the community?
- What exactly is needed to solve this problem?
- Why their method will work, and other methods will (or did) not work?

The pitches will be an opportunity to reflect on the challenges chosen by the research groups and connect directly to the NABC session. The NABC session will be further exploited during the Thursday parallel session.

On Thursday (09.00-16.00) the participants in groups will focus on drafting a very-short joint research proposal to funding agencies (max one-page-long), and then will prepare a short 5-min pitch presenting the proposal. The groups may use what they have learned during the NABC workshop the day before. The proposal may use, for example, the four NABC fundamentals to define the projects' value: "Need", "Approach", "Benefits", and "Competition/alternatives".

The Thursday session will end up with an evaluation. The groups will submit the proposal text to the moderator who will then redistribute the texts to evaluating groups. After lunch, the



MIRAI Scientific Session,  
13-14 November 2019,  
Stockholm, Sweden

groups will present the proposals during 5-min pitches. The proposal texts shall be handed in to the moderator group before noon, an hour before the pitches. The evaluating group will provide the first feedback and evaluate the proposed project right after the pitch. Each group will contribute to the session with a pitch and evaluation, everyone will be allowed to question the projects, but the evaluators will do it first.

Stockholm: Wednesday, Nov 13 <sup>th</sup> .			Location
08.00	Pick up at recommended hotels		
08.30 – 08.40	Opening Remarks/Welcome	Prof. Kazuhiro Ema, Sophia University and Dr. Piotr Matyba, Umeå University	Session rooms at Aula Magna Stockholm University
08.40 – 09.20	<b>Keynote Japan:</b> Professor Takashi Hayashita, Sophia University	Design of Novel Supramolecular Analytical Reagents for Ion and Molecule Recognition in Water	
09.20 – 10.00	<b>Keynote Sweden:</b> Professor Anders Nilsson Stockholm University	Catalysis for a Sustainable Society	
10.00 – 10.20	Fika & Photo		Outside Aula Magna
10.20 – 10.25	Introduction to presentations (Dr. Piotr Matyba, Umeå University)		Aula Magna
10.25 – 11.25	<b>Pitch presentations</b> by new members (11 persons x 3 min/person). All researchers who have been to previous MIRAI workshops get 1 ppt slide shown based on the abstract they have submitted.		Aula Magna
11.25 – 11.30	Intro to the Group Session	Prof. Kazuhiro Ema, Sophia University and Dr. Piotr Matyba, Umeå University	Session rooms at Aula Magna
11.30 – 12.20	<b>Group Session:</b> Work in Swedish-Japanese teams.		Session rooms at Aula Magna
	<b>Goal:</b> Define a research problem for the proposal writing and then prepare a 5-minutes-long pitch to present the problem to all other groups.		
12.20 – 13.10	Lunch		TBA
13.10 – 14.00	<b>Group Session, continued:</b> Work in Swedish-Japanese teams. Goal: Define a research problem for the proposal writing and then prepare a 5-minutes-long pitch to present the problem to all other groups.		Session rooms at Aula Magna
14.00 – 14.20	Fika		

14.20 – 15.20	<b>Pitch Session:</b> Each team presents the problem they chose to solve jointly. A 5-min pitch is followed by questions from the audience. <b>Moderator:</b> Professor Kazuki Sada, Hokkaido University		Session rooms at Aula Magna
15.30 – 18.30	<b>Joint workshop: “From research to societal impact: The NABC method”</b>  <u>Background:</u> The NABC method was developed by the Stanford Research Institute many years ago. Since then millions of researchers all over the world have used the method to present their research in an easy-to-understand way. This is your opportunity to learn how to communicate the value of your research and avoid rejections based on incomprehension.		Session rooms at Aula Magna
19.00 – 21.30	Reception hosted by the City of Stockholm		Stockholm City Hall
<b>Stockholm: Thursday, Nov 14<sup>th</sup>.</b>			<b>Location</b>
09.00 – 09.10	<b>Opening:</b> Summary of the previous day & intro to the Group Session	Prof. Kazuhiro Ema, Sophia University and Dr. Piotr Matyba, Umeå University	Session rooms at Aula Magna Stockholm University
09.20 – 11.50	<b>Group Session:</b> Work in the Swedish-Japanese teams.		Session rooms at Aula Magna
	<b>Goal:</b> Draft a one-page-long proposal and prepare a 5-min-long pitch for the after-lunch session. Submit the proposal draft to the moderator (Dr. Piotr Matyba).  <b>Fika</b> will be around 10:00-10:20.		
11.50 – 12.20	<b>Group Session:</b> Reading 1-page proposals		Session rooms at Aula Magna
12.30 – 13.30	Lunch		TBA
13.40 – 16.00	<b>Pitch Session:</b> Each team presents the research proposal. A 5-min pitch followed by questions from the evaluating group, and then from the audience (10 min per pitch incl. questions). <b>Moderator:</b> Professor Yasuchika Hasegawa, Hokkaido University  <b>Fika</b> will be around 14:40-15:00.		Session rooms at Aula Magna



MIRAI Scientific Session,  
13-14 November 2019,  
Stockholm, Sweden

16.15 – 17.00	Reporting from the parallel sessions. Closing speech by President Astrid Söderbergh Widding, Stockholm University.	Session rooms at Aula Magna
18.00	Farewell Reception hosted by the Embassy of Japan	Residence of the Japanese Ambassador, Djursholm, Stockholm

## KEYNOTE SPEAKER JAPAN

### Design of Novel Supramolecular Analytical Reagents for Ion and Molecule Recognition in Water

Takashi Hayashita

*Department of Materials and Life Sciences, Faculty of Science and Technology,  
Sophia University, Tokyo 102-8554, Japan  
ta-hayas@sophia.ac.jp*

The selective transduction of molecular recognition events into physical or chemical signals is a key concept for the design of novel supramolecular sensors. Various combinations of fluorescent probes and azoprobes possessing the binding sites of phenylboronic acids and dipicolyl amines with cyclodextrins (CyDs), the unique recognition functions for sugars, metal ions, and phosphate derivatives were performed by CyD complexes, chemically modified CyD complexes, and CyD gel complexes based on their synergistic functions. To realize a novel supramolecular chirality, the twisted structure of ditopic azoprobes inside the CyD was successfully controlled by multi-point recognition of guest ions in water<sup>9</sup>. The CyD nanogels and dendrimer nanoparticles having phenylboronic acid binding sites were found to discriminate the species of bacteria. These unique functions of supramolecular CyD complexes and nanogel sensors are discussed in relation to the water safety of human life based on SDG goals of #6.

## KEYNOTE SPEAKER SWEDEN

### Catalysis for a Sustainable Society

Anders Nilsson

*Division of Chemical Physics, Department of Physics, AlbaNova University Center, Stockholm  
University, SE-106 91 Stockholm, Sweden*

One of the most important current challenges in our society today is to mitigate climate change. Although wind and solar energy are becoming cheaper than fossil sources for electricity production there is a severe issue with energy storage when the wind is not blowing or the sun is not shining. We are still far from electrifying our transport sector and electrical vehicles comes also with its own environmental impact. Furthermore, the chemical and fuel industrial sector accounts for one seventh of the current greenhouse gas emission. There is a need to convert the whole chemical industry from instead relying on fossil sources to use the cheap electricity from solar and wind. Maybe there is also an opportunity with negative emissions by converting already emitted CO<sub>2</sub> to useful chemicals and materials. The key in this transformation is finding new catalysts that can form the basis for a new industry. I will in this talk present the need for material discovery of new catalysts and how x-rays at synchrotron radiation and x-ray laser sources can be essential in this development.



MIRAI Scientific Session,  
13-14 November 2019,  
Stockholm, Sweden

## **NEW MEMBERS**

## Optical properties of perovskite materials and contamination control for spacecrafts using photocatalysts

Naoki Shimosako

Faculty of Science and Technology, Sophia University, Japan  
n-shimosako2k0@sophia.ac.jp



Organic-inorganic metal halides perovskite materials have attracted interest for solar cells because of its low cost of production, high absorption, light weight, and high emission efficiency. The photo-conversion efficiency of perovskite solar cells has already reached over 20% in only several years [1]. The basic optical properties of perovskite materials have not been clear while the developments of perovskite solar cells have been conducted actively. For perovskite solar cells with high efficiency, understanding their properties are necessary. We have studied their fundamental optical properties using photoluminescence (PL) and time-resolved PL measurements [2, 3].

Optical measurements from satellites are effective to monitor global environment and study astrophysics. However, it has been reported that contamination outgassed from spacecraft's materials can degrade optical devices (mirrors, lens, filters and so on) mounted spacecrafts in orbit [4]. Solving the contamination problem is important because it influences the success of spacecraft missions. We have focused on photocatalysis materials as a new method to remove contamination in orbit. However, space environment may have negative effect on photocatalytic activity. We have studied the effect of space environment on photocatalytic activity of  $\text{TiO}_2$  to develop photocatalyst working in space [5–7].

### References

- [1] Research Cell Efficiency Record, Nation Renewable Energy Laboratory (NREL).
- [2] H. Kunugita, Y. Kiyota, Y. Udagawa, Y. Takeoka, Y. Nakamura, J. Sano, T. Matsushita, T. Kondo, and K. Ema, *Jpn. J. Appl. Phys.* 55, 060304 (2016).
- [3] H. Kunugita, T. Hashimoto, Y. Kiyota, Y. Udagawa, Y. Takeoka, Y. Nakamura, J. Sano, T. Matsushita, T. Kondo, T. Miyasaka, and K. Ema, *Chem. Lett.* 44, 852 (2015).
- [4] A.C. Tribble, *Fundamentals of Contamination Control*, Vol. TT44 SPIE Publications (2000).
- [5] N. Shimosako, K. Yoshino, K. Shimazaki, E. Miyazaki, and H. Sakama, *Thin Solid Films* 686, 137421 (2019).
- [6] N. Shimosako, Y. Hara, K. Shimazaki, E. Miyazaki, and H. Sakama, *Acta Astronaut.* 146, 1 (2018).
- [7] N. Shimosako, T. Egashira, K. Yoshino, K. Shimazaki, E. Miyazaki, and H. Sakama, *Proc. SPIE* 10748, 1074810 (2018).

## Resolving structural dynamics of liquid water using coherent x-ray sources

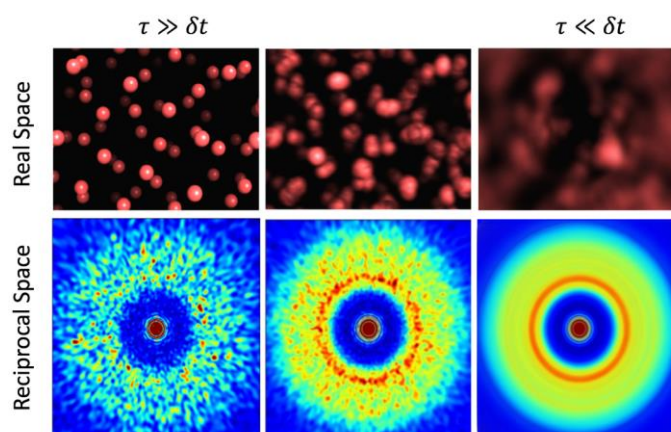
Foivos Perakis

Physics Department, Stockholm University  
[f.perakis@fysik.su.se](mailto:f.perakis@fysik.su.se)



Resolving structural dynamics is of fundamental importance to many processes across fields, ranging from material science to biophysics. Here, I will present the application of a novel coherent scattering technique that goes beyond the pump-probe scheme and enables measuring non-equilibrium structural dynamics, called X-ray Photon Correlation Spectroscopy (XPCS) (Fig. 1). The experiments utilize novel coherent x-ray diffraction techniques in new x-ray sources, such as the x-ray synchrotrons and X-ray Free-Electron Lasers. In recent XPCS experiments, we were able to probe water dynamics on the order of seconds at synchrotrons<sup>1</sup> and on the order of femtoseconds at free-electron lasers<sup>2</sup>.

These revolutionary new tools can become extremely useful for capturing in-situ the water-salt separation upon freezing which occurs during freeze-desalination. Our studies<sup>3</sup> indicate that one of the limitations of this desalination approach is that salt can be trapped inside the ice in the form of impurities. Thereby, being able to observe the water-salt separation on a molecular level can shed light to the technical limitations of the different technologies and allow the improvement of the desalination efficiency, which is directly related to SDG goal #6 aiming to boost the development of water related technologies, such as desalination and purification.



**Fig. 1** X-ray Photon Correlation Spectroscopy (XPCS) allows probing dynamics from femtoseconds to seconds with variable length-scale sensitivity from atomic scales to the mesoscale. The motion in real space (upper) is reflected in the speckle pattern (lower) in reciprocal space.

### References

1. F. Perakis, K. Amann-Winkel, F. Lehmkuhler, M. Sprung, D. Mariedahl, J. A. Sellberg, H. Pathak, A. Späh, F. Cavalca, D. Schlesinger, A. Ricci, A. Jain, B. Massani, F. Aubree, C. J. Benmore, T. Loerting, G. Grübel, L. G. M. Pettersson and A. Nilsson, Diffusive dynamics during the high-to-low density transition in amorphous ice, *PNAS*, 2017, **114**, 8193–8198.
2. F. Perakis, G. Camisasca, T. J. Lane, A. Späh, K. T. Wikfeldt, J. A. Sellberg, F. Lehmkuhler, H. Pathak, K. H. Kim, K. Amann-Winkel, S. Schreck, S. Song, T. Sato, M. Sikorski, A. Eilert, T. McQueen, H. Ogasawara, D. Nordlund, W. Roseker, J. Koralek, S. Nelson, P. Hart, R. Alonso-Mori, Y. Feng, D. Zhu, A. Robert, G. Grübel, L. G. M. Pettersson and A. Nilsson, Coherent X-rays reveal the influence of cage effects on ultrafast water dynamics, *Nature Communications*, 2018, **9**, 1917.
3. I. Tsironi, D. Schlesinger, A. Späh, L. Eriksson, M. Segad and F. Perakis, Brine rejection and hydrate formation during freeze desalination, *arXiv:1904.03682 [physics]*.

## Plasma spray for industry compatible production of nanostructured materials for high density energy storage

Dr. Makoto Kambara, Associate Professor  
*Department of Materials Engineering, The University of Tokyo, Japan*  
*mkambara@plasma.t.u-tokyo.ac.jp*



### Abstract

Nanocomposite Si particles are known as a key to attain high cycle capacities for next-generation high density lithium-ion batteries [1-3]. The battery industries yet seek for a method to produce such composites from low cost feedstocks at higher throughputs to meet ever-increasing demands from the market. In this aspect, plasma spray, a method to produce nanoparticles from powder feedstocks, could be one potential candidate; in fact we have produced various nanoparticles (NP) and demonstrated appreciable increase in cycle capacities while maintaining high throughputs [4-7]. Example structures are Si-NP with carbon coating and Si-NP attached with Ni-NP having unique epitaxial  $\text{NiSi}_2$  interfaces, both of which result in an increased cycle capacities.  $\text{SnO}$  coating on Si-NP facilitates low temperature disproportionation reaction to configure fine nanocomposite structures and attains significantly high cyclability owing to conversion reaction. Further structural modification such as one dimensional nanorod is also made possible by a control of co-condensation in the plasma flame to attain the requirements for VLS of nanowire growth. As such, plasma spray offers various opportunities to produce unique nanomaterials for future storage devices at high throughputs. In the presentation, details of the co-condensation steps and the potentials for various batteries will be presented.

### References

- [1] Graetz, J., Ahn, C. C., Yazami, R. & Fultz, B. Highly Reversible Lithium Storage in Nanostructured Silicon. *Electrochem. Solid-State Lett.* 6, A194 (2003).
- [2] Liu, X. H. et al. Size-Dependent Fracture of Silicon Nanoparticles During Lithiation. *ACS Nano* 6, 1522–1531 (2012).
- [3] Magasinski, A. et al. High-performance lithium-ion anodes using a hierarchical bottom-up approach. *Nat. Mater.* 9, 353–358 (2010).
- [4] Kambara, M. et al. Nano-composite Si particle formation by plasma spraying for negative electrode of Li ion batteries. *J. Appl. Phys.* 115, 143302 (2014).
- [5] Homma, K., Kambara, M. & Yoshida, T. High throughput production of nanocomposite  $\text{SiO}_x$  powders by plasma spray physical vapor deposition for negative electrode of lithium ion batteries. *Sci. Technol. Adv. Mater.* 15, 025006 (2014).
- [6] Fukada, K., Ohta, R. & Kambara, M. Enhanced Cycle Capacity of Lithium Ion Batteries with Nanocomposite Si Anodes Produced By Rapid Co-Condensation in Plasma Spray PVD. *ECS Trans.* 77, 41–47 (2017).
- [7] Ohta, R., Fukada, K., Tashiro, T., Dougakiuchi, M. & Kambara, M. Effect of PS-PVD production throughput on Si nanoparticles for negative electrode of lithium ion batteries. *J. Phys. D: Appl. Phys.* 51, 105501 (2018).

## Amorphous magnets

Petra Jönsson

*Department of Physics and Astronomy, Uppsala University, Sweden*  
*petra.jonsson@physics.uu.se*



### Abstract

In the electrical energy system, there is a huge potential for reducing energy losses if replacing the transformer steel used today with better soft magnetic material. For permanent magnets, the challenge is to find rare earth lean materials with magnetic properties that match those of the permanent magnets used today. Another class of magnetic materials, that could be used for energy-efficient cooling devices, are those exhibiting a strong magnetocaloric effect close to room temperature. Amorphous magnets are interesting for energy applications because of their lack of magnetocrystalline anisotropy and the endless possibilities to tune their magnetic properties by varying the composition. We use combinatorial magnetron sputtering to make compositionally graded thin film samples to find optimized compositions [1]. We also use ion-implantation in combination with lithographically produced masks to locally change the composition of an amorphous material to create magnetic composite structures on the meso or nanoscale [2]. Additive manufacturing could be a possible route to producing large sized amorphous materials with geometrical shapes impossible to produce with traditional production methods.

### References

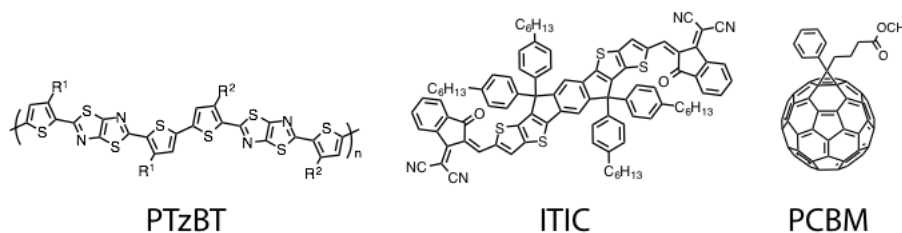
1. A. Frisk, M. Ahlberg, G. Muscas, S. George, R. Johansson, W. Klysubun, P. E. Jönsson, and G. Andersson, *Phys. Rev. Materials* 3, 074403 (2019)
2. G. Muscas, R. Brucas, and P. E. Jönsson, *Phys. Rev. B* 97, 174409 (2018)

## Efficient ternary blend solar cells with a very small amount of third component

Dr. Masahiko Saito, Assistant Professor  
Department of Applied Chemistry, Hiroshima University, Japan  
[masahikosaito@hiroshima-u.ac.jp](mailto:masahikosaito@hiroshima-u.ac.jp)



In the last decade, significant improvement of the power conversion efficiency has been made in organic photovoltaics (OPVs) [1-3]. OPV is generally based on bulk-heterojunction (BHJ) structure consisting p-type polymers and fullerene derivatives or non-fullerene small molecular compounds as n-type materials. Ternary blend cells, in which three organic semiconductors are blended to efficiently absorb broad ranges of the incident light, have shown to be a good strategy for improving the efficiency.[4,5] Here, we show that a ternary system composed of a thiazolothiazole-thiophene polymer (PTzBT)[6-8] and PCBM with a small amount (ca. 6 wt%) of ITIC[9] as the third component greatly improved the efficiency up to 10.3% ( $J_{SC} = 16.5 \text{ mAcm}^{-2}$ ,  $V_{OC} = 0.89 \text{ V}$ ,  $FF = 0.70$ ) from those of the PTzBT:PCBM binary system (7.5%:  $J_{SC} = 11.3 \text{ mAcm}^{-2}$ ,  $V_{OC} = 0.87 \text{ V}$ ,  $FF = 0.76$ ). Furthermore, modification of the polymer structure has led to the efficiency close to 11%. We note that this is probably the smallest third component ratio for ternary blend cells that exhibit efficiencies over 10%. Interestingly, although this ternary blend system included only 6 wt% of ITIC, the external quantum efficiency at the ITIC absorption was similar to that at the polymer absorption. In addition, optimal active layer thickness of the PTzBT:PCBM:ITIC ternary blend cells was as thick as 370 nm



### References

1. Zhao, W.; Li, S.; Yao, H.; Zhang, S.; Zhang, Y.; Yang, B.; Hou, J., *J. Am. Chem. Soc.* **2017**, *139* (21), 7148-7151.
2. Yuan, J.; Zhang, Y.; Zhou, L.; Zhang, G.; Yip, H.-L.; Lau, T.-K.; Lu, X.; Zhu, C.; Peng, H.; Johnson, P. A.; Leclerc, M.; Cao, Y.; Ulanski, J.; Li, Y.; Zou, Y., *Joule* **2019**, *3* (4), 1140-1151.
3. Cui, Y.; Yao, H.; Zhang, J.; Zhang, T.; Wang, Y.; Hong, L.; Xian, K.; Xu, B.; Zhang, S.; Peng, J.; Wei, Z.; Gao, F.; Hou, J., *Nature Commu.* **2019**, *10* (1), 2515.
4. An, Q.; Zhang, F.; Zhang, J.; Tang, W.; Deng, Z.; Hu, B., *Energy & Environ.l Sci.* **2016**, *9* (2), 281-322.
5. Huang, H.; Yang, L.; Sharma, B., *J. Mater. Chem. A* **2017**, *5* (23), 11501-11517.
6. Osaka, I.; Saito, M.; Mori, H.; Koganezawa, T.; Takimiya, K., *Adv. Mater.* **2012**, *24* (3), 425-430.
7. Osaka, I.; Saito, M.; Koganezawa, T.; Takimiya, K., *Adv. Mater.* **2014**, *26* (2), 331-338.
8. Saito, M.; Koganezawa, T.; Osaka, I., *ACS Appl. Mater. & Interfaces* **2018**, *10* (38), 32420-32425.
9. Lin, Y.; Wang, J.; Zhang, Z.-G.; Bai, H.; Li, Y.; Zhu, D.; Zhan, X., *Adv. Mater.* **2015**, *27* (7), 1170-1174.

## **Ion Mobility Mass Spectrometry for the Rapid Determination of the Topology of Interlocked and Knotted Molecules**

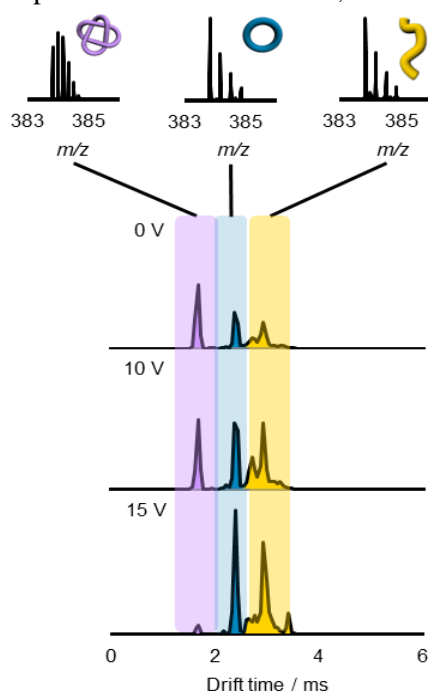
Anneli Kruve  
Stockholm University, ACES  
[Anneli.kruve@aces.su.se](mailto:Anneli.kruve@aces.su.se)



### **Abstract**

Interlocked and knotted structures are familiar in our everyday life; examples range from shoe laces and chains to symbols in art carved into stone in ancient times.[1] Molecular knots are topologically complex, self-entwined rings, while catenanes, in topology also called links, are structures formed by at least two mechanically interlocked rings. Molecular knots and catenanes were discovered already decades ago; for example, bacteriophages pack DNA with almost the density of crystals by making use of knotted structures.[2] Knots and catenanes have also become an important research field in supramolecular chemistry, not only motivated by the beauty of their structures, but also by their use as molecular machines.[3,4]

Here we present a rapid screening method based on traveling-wave ion mobility spectrometry (TWIMS) combined with tandem mass spectrometry provides insight into the topology of interlocked and knotted molecules, even when they exist in complex mixtures such as interconverting dynamic combinatorial libraries. A TWIMS characterization of structure-indicative fragments generated by collision-induced dissociation (CID) together with a floppiness parameter defined merely based on parent and fragment ion arrival times provide a straightforward topology identification. To demonstrate its broad applicability, this approach is applied here six Hopf and two Solomon links, a trefoil knot, and a [3]catenate.

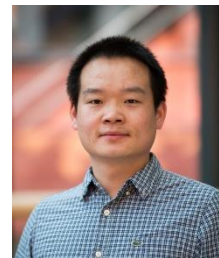


### **References**

1. C. J. Bruns, J. F. Stoddart, in *Beauty Chem.* (Ed.: L. Fabbriizzi), Springer Berlin Heidelberg, Berlin, Heidelberg, 2011, pp. 19–72.
2. J. Arsuaga, M. Vazquez, P. McGuirk, S. Trigueros, D. W. Sumners, J. Roca, *Proc. Natl. Acad. Sci.* 2005, 102, 9165–9169.
3. J.-F. Ayme, J. E. Beves, C. J. Campbell, D. A. Leigh, *Angew. Chem. Int. Ed.* 2014, 53, 7823–7827.
4. N. H. Evans, *Chem. - Eur. J.* 2018, 24, 3101–3112

## Single crystalline NMC cathode materials to enable long-life lithium ion batteries

Dr. Haidong Liu, Postdoctoral researcher  
*Department of Chemistry-Ångström Laboratory, Uppsala University*  
*Haidong.liu@kemi.uu.se*



### Abstract

Layered Ni-rich  $\text{LiNi}_x\text{Mn}_y\text{Co}_{1-x-y}\text{O}_2$  ( $x > 0.5$ , NMC) materials have attracted intensive attention to develop high energy-density lithium ion batteries, owing to the high capacity and relatively low cost. However, the limited cycle life is becoming the plague of the practical application due to the structural instability, microcracks formation and interfacial side reactions at high voltage. To overcome these issues, single crystalline Ni-rich materials with a large particle size of around 5  $\mu\text{m}$  and polyhedral shape were synthesized. Meanwhile, in order to alleviate the surface side reaction with electrolyte at high cut-off voltage, a homogeneous ultrathin  $\text{Al}_2\text{O}_3$  layer ( $\sim 2$  nm) was coated on the surface of the single crystal materials. Compared with the conventional polycrystalline spherical NMC cathode materials, the single crystalline NMC materials can provide a more stable surface activity resulting from the low surface area and better mechanical stability. Moreover, single crystal NMC materials have higher energy density due to the increased tap density than the conventional polycrystalline spherical NMC materials. As a result, a higher reversible capacity and significant improvement of cycling stability were realized. The structure, surface stability and electrochemical performance of the single crystalline NMC with  $\text{Al}_2\text{O}_3$  coating have been investigated in details.

### References

- [1] H. Y. Li, J. Li, X. W. Ma, J. R. Dahn. *J. Electrochem. Soc.* 2018, 165, A1038-A1045.
- [2] J. Kim, H. Lee, H. Cha, M. Yoon, M. Park, J. Cho. *Adv. Energy Mater.* 2018, 8, 1702028.
- [3] H. D. Liu, R. Kloepsch, J. Wang, M. Winter, J. Li. *J. Power Sources* 2015, 300, 430-437.
- [4] H. D. Liu, J. Wang, X. F. Zhang, D. Zhou, X. Qi, B. Qiu, J. H. Fang, R. Kloepsch, G. Schumacher, Z. P. Liu et al. *ACS Appl. Mater. Interfaces* 2016, 8 (7), 4661-4675.

## Two-dimensional mutually synchronized spin Hall nano-oscillator arrays for highly coherent microwave signal generation and neuromorphic computing

Dr. Johan Åkerman, Professor  
*Department of Physics, University of Gothenburg*  
*johan.akerman@physics.gu.se*



### Abstract

Mutually synchronized spin torque nano-oscillators (STNOs) are one of the promising platforms for bioinspired computing and microwave signal generation [1, 2]. Using STNOs one can achieve 90% recognition rate in spoken vowels [3]. However, in order to do more complex tasks, larger scale synchronized oscillators are needed, something that is not easily done with the STNOs demonstrated so far.

In my talk, I will describe a different type of spin current driven device called spin Hall nano-oscillators (SHNOs), which can generate microwave frequencies over a very wide frequency range [4]. The SHNOs are based on 50 – 120 nm wide nano-constrictions in Pt(5)/Hf(0.5)/NiFe(3) trilayers (all numbers in nm). When multiple nano-constrictions are fabricated close to each other (300 – 1200 nm separation) they can mutually synchronize and chains of up to nine nano-constrictions have been demonstrated to exhibit complete synchronization [5]. For the first time, we can now also synchronize two-dimensional SHNO arrays with as many as  $8 \times 8 = 64$  SHNOs [6]. The mutual synchronization is observed both electrically and using scanning micro-BLS microscopy. Both the output power and linewidth of the microwave signal improves substantially with increasing number of mutually synchronized SHNOs, such that quality factors of about 170,000 can be reached. Following the approach of Romera et al [3], we also demonstrate neuromorphic computing using a  $4 \times 4$  SHNO array with two injected microwave signals as inputs.

Given their high operating frequency (~10 GHz), easy fabrication, and highly robust synchronization properties, nano-constriction SHNO arrays are likely the most promising candidates for neuromorphic computing based on oscillator networks.

### References

- [1] J. Grollier, D. Querlioz, and M. D. Stiles, *Proc. IEEE* **104**, 2024 (2016).
- [2] J. Torrejon et al, *Nature* **547**, 428 (2017)
- [3] M. Romera et al, *Nature* **563**, 230–234 (2018)
- [4] T. Chen, R. K. Dumas, A. Eklund, P. K. Muduli, A. Houshang, A. A. Awad, P. Dürrenfeld, B. G. Malm, A. Rusu, and J. Åkerman, *Proc. IEEE* **104**, 1919 (2016)
- [5] A. A. Awad, P. Dürrenfeld, A. Houshang, M. Dvornik, E. Iacocca, R. K. Dumas, and J. Åkerman, *Nature Physics* **13**, 292–299 (2017)
- [6] M. Zahedinejad, et al. arXiv:1812.09630 (2018); *Nature Nanotechnology*, *accepted* (2019)

## Understanding and controlling the epitaxial growth of 2D heterostructures (via *in situ* TEM)

Dr. Hamid Reza Barzegar, Senior Research assistance  
Department of Physics, Umeå University, Sweden



The quick expansion of the two-dimensional (2D) material library raises several fundamental scientific questions as well as remarkable opportunities for technological applications. In addition, 2D materials have a unique degree of freedom, namely the ability to form heterostructures by stacking different 2D materials on top of each other (vertical heterostructure), or in-plane interconnected structures (in-plane heterostructure). The vertical heterostructures may form by epitaxial growth in which the growth of the top layer is influenced by the underneath layer structural properties. In the last decade the growth dynamic of graphene on different substrates have been extensively studied. However there is lack of information on the growth kinetic of the more recently developed 2D materials such as atomically thin transition metal dichalcogenide (TMD). Since TMDs have several potential applications in electronic devices, the controlled growth of their atomically thin layers as well as heterostructures are of significant importance. Yet the mechanism of the crystal phase formation and transformation is not clear and there are lots of complexities on the epitaxial growth of recent TMD heterostructures. We are planning to increase understanding of the epitaxial growth of 2D heterostructures via *in situ* transmission electron microscopy (TEM) experiments in which the dynamics of the atoms in top layer are tracked at elevated temperatures and under the influence of the underneath layer material. The outcome of the experiment, in combination with theoretical analysis, will be used to understand the growth dynamic of the desired material. Moreover the result can be employed to tune the properties of the heterostructures for further application in different fields.

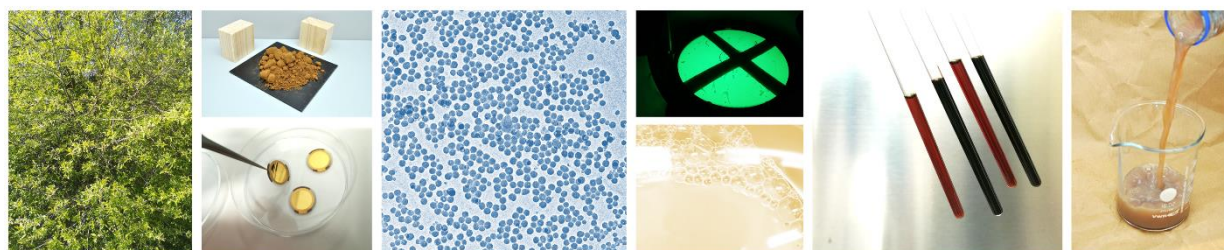
## Sustainable materials from lignin

Mika Sipponen, D.Sc. (Tech.), Assistant Professor  
*Department of Materials and Environmental Chemistry, Stockholm University*  
[mika.sipponen@mmk.su.se](mailto:mika.sipponen@mmk.su.se)



### Abstract

Lignins are C-C and C-O-C interlinked p-hydroxyphenyl propanoids. This group of polyphenols is the second most abundant natural polymer and the main polyphenol component of terrestrial plant biomass. Millions of tons of lignin is separated from the forest and agro biomass every year, but most of this lignin is not used in materials but is instead combusted for energy. Promisingly, the past five years have seen a paradigm shift in the efforts to utilize lignin in materials. In addition to carbon fixation in lignin-based materials, which itself contributes to the carbon-neutral society, there are many opportunities to harness the intrinsic properties of lignin in matching applications. Especially the advent of lignin nanoparticles (LNPs) has opened new ways to benefit from lignins' barrier properties,<sup>[1]</sup> surface activity,<sup>[2-4]</sup> antioxidant activity<sup>[5]</sup> and encapsulation of active ingredients.<sup>[5-7]</sup> These spherical particles can be produced from a variety of different lignins, overcoming their structural complexity in the form of standardized building blocks. This presentation gives a current outlook of the opportunities and challenges of lignin in sustainable material applications. In addition,



### References

1. Farooq, M., Zou, T., Riviere, G., Sipponen, M.H. & Österberg, M. Strong, ductile and waterproof cellulose nanofibril composite films with colloidal lignin particles. *Biomacromolecules* 20, 693–704 (2019).
2. Sipponen, M.H. et al. Spatially confined lignin nanospheres for biocatalytic ester synthesis in aqueous media. *Nat. Commun.* 9, 1–7 (2018).
3. Sipponen, M. H., Smyth, M., Leskinen, T., Johansson, L.-S. & Österberg, M. All-lignin approach to prepare cationic colloidal lignin particles: Stabilization of durable Pickering emulsions. *Green Chem.* 19, 5831–5840 (2017).
4. Zou, T., Sipponen, M.H. & Österberg, M. Natural shape-retaining microcapsules with shells made of chitosan- coated colloidal lignin particles. *Front. Chem.* 7, 2300 (2019).
5. Sipponen, M.H., Lange, H., Ago, M. & Crestini, C. Understanding Lignin Aggregation Processes. A Case Study: Budesonide Entrapment and Stimuli Controlled Release from Lignin Nanoparticles. *ACS Sustainable Chem. Eng.* 6, 9342–9351 (2018).
6. Sipponen, M.H., Lange, H., Crestini, C., Henn, A. & Österberg, M. Lignin for nano- and microscaled carrier systems: applications, trends and challenges. *ChemSusChem* 12, 2039–2054 (2019).
7. Figueiredo, P., Sipponen, M.H., Preparation and Characterization of Dentin Phosphophoryn-Derived Peptide-Functionalized Lignin Nanoparticles for Enhanced Cellular Uptake. *Small* 15: 1901427 (2019).
8. Sipponen, M.H. & Österberg, M. Aqueous Ammonia Pre-treatment of Wheat Straw: Process Optimization and Broad Spectrum Dye Adsorption on Nitrogen-Containing Lignin. *Front. Chem.* 7, 1–14 (2019).
9. Sipponen, M.H., Henn, A., Penttilä, P., Österberg, M. Lignin-fatty acid hybrid nanocapsules for thermal energy storage in phase-change materials. Submitted

## Lead-Free Double Perovskites and Their Optoelectronic Properties

Feng Wang, Assistant Professor  
Department of Physics, Chemistry and Biology (IFM)  
feng.wang@liu.se

### Abstract

Solar cells are considered as one of the promising renewable energy sources for the rising world energy demand by converting sunlight into electricity. Lead halide perovskites ( $\text{APbX}_3$ , where A is inorganic cesium or an organic cation, B site is Pb and X is a halide anion.) have shown great success in photovoltaic applications during the past few years, with a high certified power conversion efficiency of 25.3%.<sup>1</sup> Despite these exciting advances, the toxicity of lead in the materials is a crucial challenge hindering their practical applications.<sup>2</sup> Recently, we focus on a promising lead-free perovskite materials - halide double perovskites with the formula of  $\text{A}_2\text{N}^+\text{M}^{3+}\text{X}_6$ , where toxic bivalent  $\text{Pb}^{2+}$  cations are replaced by a combination of non-toxic monovalent and trivalent cations.<sup>3</sup> We revealed long carrier diffusion lengths of  $\text{Cs}_2\text{AgBiBr}_6$  double perovskites over 100 nm demonstrated the first double perovskite solar cells based on plenary structures.<sup>4</sup> Besides, we also demonstrated an exotic fully reversible thermochromism behavior of  $\text{Cs}_2\text{AgBiBr}_6$  in both single crystals and thin films.<sup>5</sup> Moreover, we found the absorption properties of  $\text{Cs}_2\text{AgBiBr}_6$  can be improved by introducing different dopants (Such as  $\text{Cu}^+$ ) into the crystal structure, implying immense opportunities of double perovskites for optoelectronic applications.<sup>6</sup>

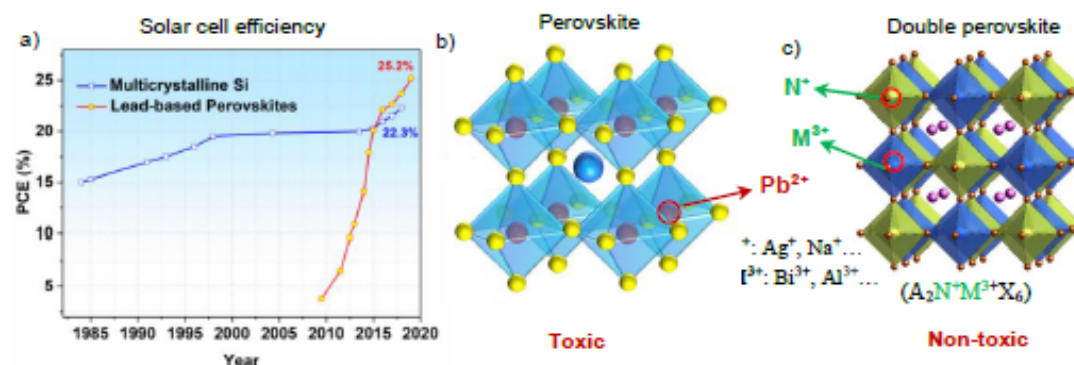


Fig. 1 a) Power conversion efficiencies of Pb-based perovskite (red line) and multicrystalline Si solar cells (blue line). b) Crystal structure of toxic lead-based perovskites. c) Crystal structure of environmentally friendly double perovskites.

### References

1. <https://www.nrel.gov/pv/cell-efficiency.html>
2. F. Wang, et al, *Advanced Functional Materials*, 2015, 26, 3417.
3. F. Giustino, et al, *ACS Energy Letter*, 2016, 1, 1233.
4. W. H. Ning, et al, *Advanced Materials*, 2018, 30, 1706246.
5. W. H. Ning, et al, *Advanced Functional Materials*, 29, 1807375 (2019)
6. F. X. Ji, et al, In prepared.