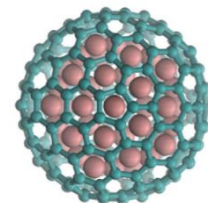


Rational design of non-noble metal (electro)catalyst materials for energy conversion applications (DEMEC)



The energy production, conversion and storage are world wide issues. The traditional energy technology based on fossil fuels cannot be used solely and new technologies are needed. The most important primary energy source is the sun. Solar energy is intermittent by nature and thus, electrical energy has to be converted and stored so that it is available when needed. In a recent report by IEA, hydrogen has been recognized as one of the best energy vectors and storage medium. Hydrogen conversion technology is in principle scalable and thus, suitable for variety of applications.

The hydrogen conversion has several problems including the storage and the fact that the commercial fuel cells and electrolyzers utilizes expensive platinum group metals (PGM) as catalysts. To cover Pt demand for very common applications, such as cars, annual Pt production should rise fivefold. Under such a high market pressure, Pt price would become astronomical limiting its use. This is one of the key problems in the hydrogen utilization and the topic of the DEMEC project.



In the DEMEC project, new electrocatalysts enabling storing of electrical energy into chemical compounds, e.g. hydrogen, and regeneration of electricity are designed, synthesized and investigated in a rational manner. The aim is to design and develop new low cost electrocatalysts for readily scalable and integrable hydrogen energy conversion technology. These materials are free of PGMs categorized as critical raw materials. Catalyst material optimization (rational design) is realized in close collaboration between groups specialized in modelling, materials synthesis and electrocatalysis. In recent years progress in developing of PGM free materials for oxygen reduction (ORR)¹⁻³ and hydrogen evolution reactions (HER)⁴ has taken place. These two are fundamentally important reaction for electrochemical energy conversion as the former reaction is met in fuel cell cathodes while the latter is one occurs in electrolysis when hydrogen is generated from water.

Recently we have shown that metal free nitrogen doped carbon nanotubes (N-CNT) are good catalyst for HER. To our knowledge this is the first time as N-CNT material is used for HER. We have also very promising results from metal capsulated systems as catalyst: Fe-CNT materials developed by us for HER are at least as good electrocatalyst as Pt/C. This is very important result since to our knowledge this is the best PGM free catalyst for HER so far. So new fundamentally interesting findings and introduction of novel durable high-performance electrocatalyst materials are expected.

1. M. Borghei, P. Kanninen, M. Lundahl, T. Susi, J. Sainio, I. Anoshkin, A. Nasibulin, T. Kallio, K. Tammeveski, E. Kauppinen, V. Ruiz, High oxygen reduction activity of few-walled carbon nanotubes with low nitrogen content, *Applied Catalysis B: Environmental*, 158–159 (2014) 233–241, DOI: 10.1016/j.apcatb.2014.04.027.
2. P. Kanninen, M. Borghei, O. Sorsa, E. Pohjalainen, E. I. Kauppinen, V. Ruiz, T. Kallio, Highly efficient cathode catalyst layer based on nitrogen-doped carbon nanotubes for the alkaline direct methanol fuel cell, *Applied Catalysis B: Environmental* 156-157C (2014) 341-349, DOI: 10.1016/j.apcatb.2014.03.041

3. S. Ratso, I. Kruusenberg, M. Vikkisk, U. Joost, E. Shulga, I. Kink, T. Kallio, K. Tammeveski, Highly active nitrogen-doped few-layer graphene/carbon nanotube composite electrocatalyst for oxygen reduction reaction in alkaline media, *Carbon* 73 (2014) 361-370. DOI: 10.1016/j.carbon.2014.02.076
4. M. Tavakkoli, T. Kallio, O. Reynaud, A. G. Nasibulin, C. Johans, J. Sainio, H. Jiang, E. I. Kauppinen, K. Laasonen, Single shell carbon-encapsulated iron nanoparticles as an active catalyst for hydrogen evolution reaction, *Angewandte Chemie* 54 (2015) 4535-4538, DOI: 10.1002/ange.201411450.


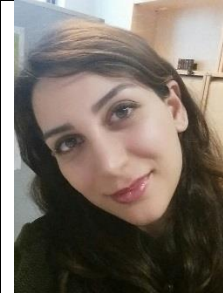
Computational chemistry

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Carbon nanomaterials

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Electrochemistry and energy conversion

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