Quantum Bio-Inorganic Chemistry Society

2020 – 2021 QBIC Society Award Symposium

5th and 7th of July 2021

In honour of the 2020 (Dr. Martin Srnec) and 2021 (Dr. Ragnar Björnsson), recipients of the QBIC Society Awards, the QBIC Society will hold a two-day mini online symposium.

We had originally anticipated that the award talks would be one of the highlights of the next QBIC meeting which was scheduled to take place at the University of Groningen, the Netherlands. Due to the unfortunate circumstances of the global pandemic, we will have to postpone the physical meeting until the world is in better shape.

The symposium will be held on the 5th and 7th of July 2021. We are delighted to have secured a number of excellent international speakers ranging from theoretical to computational, and also synthetic chemistry. The programme featuring the speaker line-up, titles of talks and times (CET) can be found below.

The online symposium will be held using Zoom. Please register here:
http://bit.ly/QBICAwards2021

Looking forward to meeting you all online.

Programme

Day I: 05.07.2021, CEST times

15.45 – 16.00	Welcome
16.00 – 16.30	Talk I: **Donald G. Truhlar**, *University of Minnesota* "Multiconfiguration Pair-Density Functional Theory: A Density Functional Method for Inherently Multiconfigurational Systems"
16.30 – 17.00	Talk II: **William B. Tolman**, *Washington University* "Proton-Coupled Electron Transfer by Copper-Oxygen Intermediates"
17.00 – 17.15	Break
17.15 – 17.45	Talk III: **Pedro Salvador**, *Universitat de Girona* "Extracting Oxidation states from electronic structure calculations."
17.45 – 18.00	Award Ceremony
18.00 – 19.00	Award Talk: **Martin Srnec** (2020), *J. Heyrovský Institute of Physical Chemistry* "Chemical Reactivity Through the Lens of Non-Traditional Concepts."

Day II: 07.07.2021, CEST times

15.45 – 16.00	Welcome
16.00 – 16.30	Talk I: **Agustí Lledós**, *Universitat Autònoma de Barcelona* "QM-based curly arrow description of reaction mechanisms"
16.30 – 17.00	Talk II: **Dennis Hetterscheid**, *Universiteit Leiden* "The Nuts and Bolts of Redox Potential Levelling in Homogeneous Catalysis".
17.00 – 17.15	Break
17.15 – 17.45	Talk III: **Anastassia N. Alexandrova**, *University of California - Los Angeles* "Intramolecular Electric Fields as Reactivity Regulator in Heme-Iron and Blue Copper Proteins."
17.45 – 18.00	Award Ceremony
18.00 – 19.00	Award Talk: **Ragnar Björnsson** (2021), *MPI for Chemical Energy Conversion* "Uncovering the electronic structure basis for biological nitrogen reduction"

Brief biography

Martin Srnec, born in 1980, grew up in Bechyně in the Czech Republic, received his Ph.D. at Institute of Organic Chemistry and Biochemistry in Prague in 2010 (with L. Rulíšek), and was a postdoctoral fellow at Stanford University in 2011-2013 (with E. I. Solomon). In 2014, he received the Purkyně fellowship from the Czech Academy of Sciences to establish his own research group at the J. Heyrovský Institute of Physical Chemistry in Prague, where he is appointed as head of the Department of Computational Chemistry from 2019. Since 2016 he also teaches at the Faculty of Science of Charles University. Dr. Srnec's research interests lie mostly in the field of theoretical bioinorganic chemistry with emphasis on the application of a range of quantum-chemical methods to elucidate geometric/electronic structure properties of various enzymatic and biomimetic redox-active transition metal sites and their contribution to reactivity, and to develop new concepts in chemical theory. He is the recipient of the Prize of Learned Society of the Czech Republic (2020), O. Wichterle premium provided by the Czech Academy of Sciences (2015), and Scopus Award for one of the three best papers published in the Czech Republic (2009).

Links: http://www.srneclab.cz

Brief biography

Credit: Thomas Hobirk, MPI-CEC

Ragnar Björnsson studied Biochemistry (B.Sc.) and Inorganic Chemistry (M.Sc.) at the University of Iceland. He obtained a PhD in Computational Chemistry in 2012 from the University of St Andrews with Prof. Michael Bühl and went on to do postdoctoral research with Prof. Frank Neese and Prof. Serena DeBeer at the Max Planck Institute for Chemical Energy Conversion. He was a research fellow at the Science Institute, University of Iceland, from 2014-2018 where he established a research group and obtained the qualification of research assistant professor. Since 2018, he is a group leader of the computational chemistry group at the Max Planck Institute for Chemical Energy Conversion. His research interests involve open-shell transition metal chemistry, environmental effects in quantum chemistry and computational spectroscopy, with biological nitrogen reduction via multiscale modelling being the main topic in the research group.

Links: https://cec.mpg.de/forschung/anorganische-spektroskopie/dr-ragnar-bjoernsson
https://sites.google.com/site/ragnarbjornsson/home