Press release
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Chao Zhang of Uppsala University receives the 2026 Arrhenius Plaque

The 2026 Arrhenius Plaque has been awarded to Chao Zhang, Senior Lecturer and Associate Professor in the Department of Chemistry – Ångström Laboratory at Uppsala University.

Chao Zhang, Uppsala University

Chao Zhang's research group is called the *TeC group* (Theory of Electrochemistry and Computation). The group develops models of electrochemical systems using atomistic simulation and machine learning.

– I am a computational chemist working mainly on electrochemical energy materials. My group uses computer simulations and, increasingly, artificial intelligence to understand what happens at the atomic and molecular level in electrochemical systems. We are particularly interested in electrolytes and electrified interfaces – in other words, how ions move through materials and liquids, and what happens where an electrolyte meets an electrode. These processes are central to batteries and many other technologies for energy storage and conversion.

One of the groups' ongoing projects is their current research on solid polymer electrolytes for next-generation batteries. These are soft materials that can conduct lithium ions and could provide safer and more sustainable alternatives to the liquid electrolytes used in many batteries today.

– The chemical space of possible polymers is enormous, so we combine molecular simulations, generative AI, and experiments to understand how these materials work and to identify promising new candidates much more efficiently.

Chao Zhang was originally trained as a materials scientist in China. He then received a generous EU scholarship to pursue a European Master's degree (Erasmus Mundus) in atomistic simulation (ATOSIM).

– I completed my PhD at RWTH Aachen University in Germany in 2013 and then worked as a postdoctoral researcher at the University of Cambridge before joining Uppsala University as an assistant professor in 2017.

How did you choose to work with electrochemistry?
– I actually came to electrochemistry almost by accident. My first PhD project involved molecular dynamics simulations of simple aqueous electrolyte solutions. My office mates were very sympathetic, because they thought the topic looked rather plain! Then I came across a monograph called Liquids, Solutions, and

Interfaces by Fawcett. It was an eye-opener. I became fascinated by the power of theory and molecular modelling to explain remarkably complex behaviour starting simply from the motions and interactions of atoms and molecules.

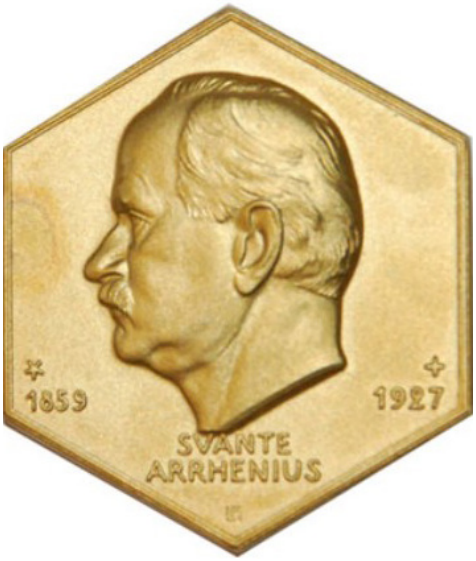
– Later, I also came to appreciate that electrochemistry is an area where fundamental physical chemistry is directly connected to important practical problems, from batteries and energy storage to electrochemical materials at large. That combination of fundamental scientific questions and real-world relevance has kept me interested ever since.

What do you enjoy most about your work?
– For me, the most enjoyable part is trying to understand something that we cannot directly see – although that also makes it rather challenging to explain to my daughter what I actually do as a scientist! Electrochemical processes often span many different length and time scales, but their behaviour ultimately emerges from the motion and interaction of atoms, molecules, ions, and electrons. With computer simulations, we can build a molecular-level picture of these processes, predict how they translate into properties that can be measured experimentally, and test why something happens.

– I also enjoy the fact that research constantly takes us in unexpected directions. Quite often, a simulation gives a result that does not fit our initial expectations. Figuring out why can be much more interesting than simply confirming what we already thought. And, of course, working with students and younger researchers and seeing them develop their own ideas is one of the most rewarding parts of the job.

How does it feel to have been awarded the Arrhenius Plaque?
– I am extremely happy and honoured to receive the Arrhenius Plaque. It means a great deal to be recognized by the Swedish Chemical Society and the Swedish chemistry community. I also see the award as recognition of the work of my whole research group and of the many students, colleagues, and collaborators I have had the privilege of working with over the years.

– It also feels particularly special because of Svante Arrhenius himself. His work on electrolytic dissociation was fundamental to our understanding of ions in solution and to the development of physical chemistry and electrochemistry. More than a century later, many of the questions my group studies are still about ions, electrolytes, and how they behave under electrical forces – although today we can investigate these processes atom by atom using computer simulations and artificial intelligence. I find that connection especially meaningful, not least given Arrhenius's strong connection to Uppsala.



About the Arrhenius Plaque (Arrhenius-plaketten)
The Arrhenius Plaque is awarded annually by the Swedish Chemical Society (Svenska Kemisamfundet) in memory of the Swedish physicist and chemist Svante Arrhenius, who was a long-time very active member of the society. The award is given to a person or persons who have distinguished themselves through outstanding research in the field of chemistry or related research fields, or who have performed valuable work for the benefit of the Swedish Chemical Society.

Contact:
Agnes Rinaldo-Matthis, Svenska Kemisamfundet
agnes.rinaldo.matthis@kemisamfundet.se

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