SUPERHEROES 4 SCIENCE

WATER DEIONIZATION

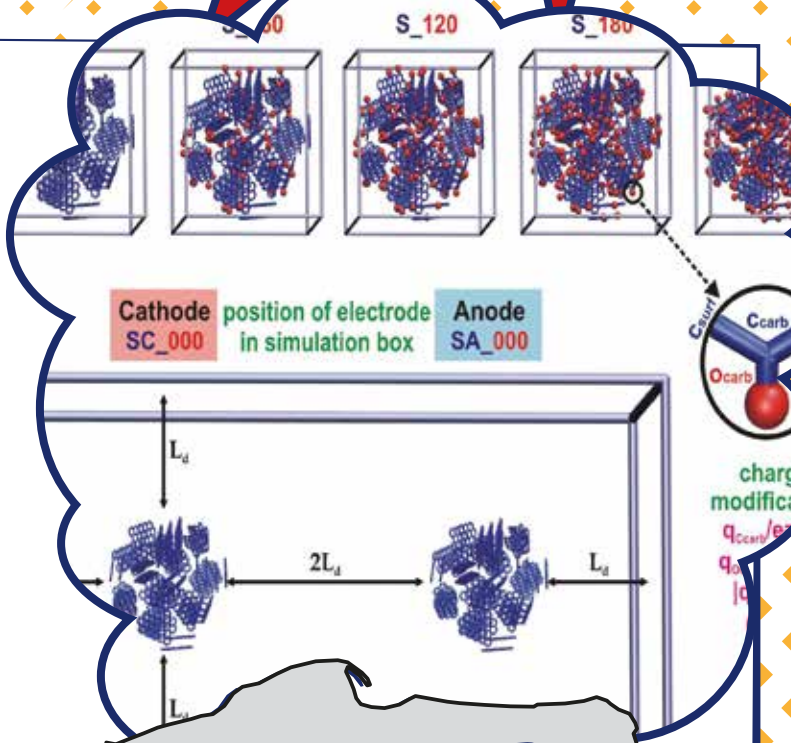
Deionization as a tool to solve the global problem of drinking water shortage

Water is one of the planet's most precious resources. According to the UNESCO 2006 UN World Water Development Report, water resources are declining and the quality of water is deteriorating in many parts of the world, while demand continues to rise. The world population is predicted to reach 8.5 billion by 2030, which will result in a 30% increase in the global demand for water, while only 60% of this demand will be met. As droughts also become more frequent, desalination of seawater will turn from an immediate measure into a long-term solution, and it is still a current subject of research in many scientific centres.

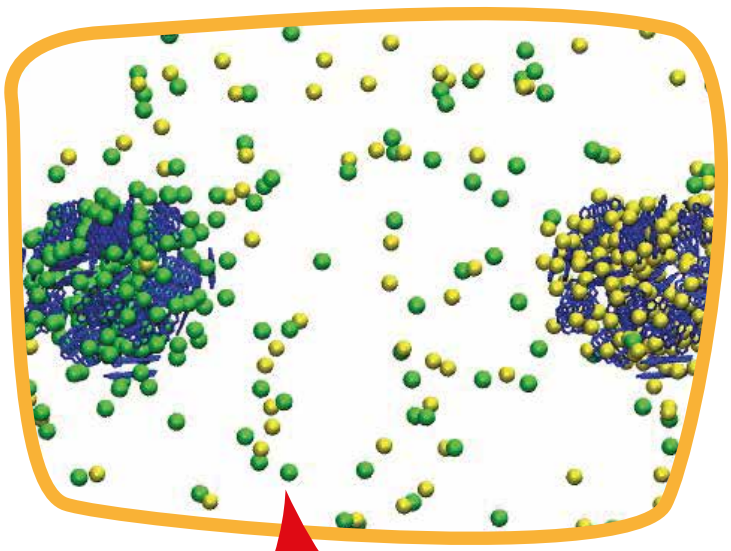
Capacitive deionization (CDI) is one of the methods for removing dissolved salts from brackish water, which is becoming a potential method for desalination of drinking water. This method is based on the accumulation of ions on the surface of electrodes under the influence of an applied electric voltage. This phenomenon is called electrosorption. The following advantages of CDI have been mentioned: no chemicals are required during the cycles of desalination and regeneration, and the applied voltages are fairly low to avoid electrolysis of the water, which make this technology non-polluting, environment-friendly, energy efficient and cost-effective for water desalination, in comparison with traditional technologies, such as thermal distillation, reverse osmosis and electrodialysis.

In recent years, there has been a rapid increase in both the scale and range of the diversity of carbon nanomaterials. The main advantage of these adsorbents is the possibility of controlled synthesis of various forms like nanotubes, nanohorns, nanoscrolls, nanocones and others. The usefulness of these materials is primarily determined by their properties (and the great opportunities to modify them) such as the developed internal surface, porous structure and chemical nature of the surface.

Since electrosorption is a surface process, one of the desirable features of electrode materials is high surface area. In addition, such a material should also be a good electric conductor. Carbonaceous adsorbents excellently meet these expectations. Hence, the determination, understanding and explanation of the regularities regarding the deionization process occurring in the pores of the carbonaceous materials are fundamental to design and optimisation of the CDI technique.



POZNAN SUPERCOMPUTING AND NETWORKING CENTER (PSNC)
www.psnc.pl



Molecular simulations are an important tool for extending our knowledge. Virtual experiments make it possible to systematically examine different combinations of factors affecting the CDI process, i.e. microstructure, surface chemistry and applied voltage. Moreover, molecular simulations give a direct insight into the mechanism of the process at the atomic level, which is impossible during typical experimental procedures.

Our research covers this area. We have used molecular dynamic simulation to determine and explain general rules determining the behaviour of ions on the charged (and uncharged) carbonaceous surfaces. We have focused among others on the effects of the chemical nature of the surface. The influence of this feature is not sufficiently known since it has often been neglected in other studies. Our studies were only possible thanks to access to the supercomputers in the Eagle cluster available at Poznan Supercomputing and Networking Center. A realistic reflection of the complex nature of the studied carbonaceous materials requires the construction of appropriately large simulations systems. This causes such simulations to become very time consuming. This fact combined with the necessity to perform simulations for many systems makes our research impossible without access to the computing power provided by the PSNC.

Dr hab. Piotr Gauden, Prof. NCU and mgr. Wojciech P. Zieliński, Faculty of Chemistry, Nicolaus Copernicus University in Torun, Gagarin St. 7, 87-100 Torun, Poland

Dr hab. Sylwester Furmaniak, Stanisław Staszic University of Applied Sciences in Piła, Podchorążych Street 10, 64-920, Piła, Poland in cooperation with Poznan Supercomputing and Networking Center, Poland

Do you want to know more?

superheroes4science.eu
facebook.com/superheroes4science
instagram.com/superheroes4science

The Superheroes 4 Science project is supported by the Visegrad Fund.
www.visegradfund.org

Visegrad Fund