Materials Science and Engineering Special Seminar

Numerical Modeling Unlocks Remarkable Ion Selectivity of Capacitive Deionization

Prof. Matthew E. Suss
Departments of Chemical and Mechanical Engineering
Technion - Institute of Technology, Haifa, Israel

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Ion-selective water treatment is an important frontier in water research, as for many applications removing all ions indiscriminately leads to significant extra energy and downstream re-ionization costs. Capacitive deionization (CDI) is under intensive investigations for ion-selective treatment of polluted feedwaters [1]. CDI has the remarkable feature of being not only highly selective, but additionally dynamically tuneable to adjust, real-time, to varying feedwater composition and produced water targets [1]. However, we will show that to further develop CDI technologies to achieve desired separations, in feedwaters of several competing anions and cations, requires detailed numerical models. Such models couple ion transport theory to nanopore electrosorption, and often include pH dynamics. We here describe our recent work exploring the limits of ion-ion selectivity by capacitive deionization with inexpensive nanoporous carbon electrodes. We show how theory enabled us to achieve in the lab remarkable selectivity and a diverse set of separations, such as "perfect" divalent cation selectivity[2], monovalent ion selectivity[3], and removal of amphoteric pollutant species such as boric acid and nutrient species[4]. We show using strong-acid functionalized electrodes that the same two-electrode system can be used for either excellent divalent selectivity, or long-lasting monovalent ion selectivity, depending on cell operational parameters [2,3]. Our work furthers the argument that membraneless CDI, based on inexpensive and easily-scalable porous carbon electrodes, can address a wide variety of important applications in water treatment.

Matthew obtained his PhD in 2013 in Mechanical Engineering from Stanford University. From 2010-2013, Matthew was a Lawrence Scholar at Lawrence Livermore National Laboratory and from 2013 to 2014 a Postdoctoral Associate in Chemical Engineering at MIT. Currently, Matthew directs the Cleantech Innovations Lab at Technion, where he is an Associate Professor affiliated with Mechani-cal Engineering, Chemical Engineering, the Grand Technion Energy Program (GTEP) and Grand Water Research Institute (GWRI).

Matthew serves as a member of the Israel National Research Center for Electrochemical Propulsion (INREP), on the European Federation of Chemical Engineering (EFCE) working group on electro-chemical engineering, and as a past Chairman of the International Working Group on Capacitive De-ionization & Electrosorption (CDI&E). Matthew is an Associate Editor with the new RSC journal Energy Advances. Matthew has co-authored over 50 journal papers in the fields of electrochemical systems theory and electrochemical energy and water systems, and is the recipient of several re-search awards including the Alon Fellowship from the Israeli government and an ARCHES award from the German government.

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[1] J.G. Gamaethiralalage, et al. "Recent advances in ion selectivity with capacitive deionization", *Energy & Environmental Science*, 2021.

[2] R. Uwayid, E.N. Guyes, A.N. Shocron, J. Gilron, M. Elimelech, M.E. Suss. "Perfect divalent cation selectivity with capacitive deionization", *Water Research*, 2022.

[3] E.N. Guyes, A. Shocron, Y. Chen, C. Diesendruck, M.E. Suss. "Long-lasting, monovalent selective capacitive deionization electrodes." *NPJ Clean Water*, 2021.

[4] A.N. Shocron, E.N. Guyes, H.H. Rijnaarts, P.M. Biesheuvel, M.E. Suss, J.E. Dykstra, "Electrochemical removal of amphoteric ions", *Proceedings of the National Academy of Sciences*, 2021.

Host: Prof. Ekaterina Pomerantseva, ep432@drexel.edu

DREXEL UNIVERSITY
College of
Engineering

FOR MORE INFORMATION

Email: kn52@drexel.edu

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