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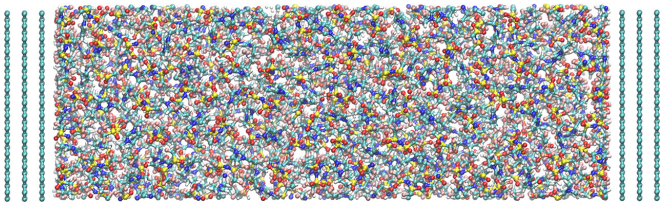
MetalWalls simulations describe the microscopic structure of battery components with classical mechanics.



In electrochemistry, potential differences drive chemical phenomena. This plays an important role in electrochemical energy storage, which is used in batteries, supercapacitors, and other devices.

Experiments can provide a macroscopic view of this technology, but examining the microscopic structure often requires accurate simulations. Such modeling can help maximize system performance by identifying the correct solvents, ions, and additives.

Coretti et al. simulated electrochemical interfaces with MetalWalls, a molecular dynamics software. By modeling the interfaces, the team hopes to provide guidance on what configurations will improve energy storage.

“The main difficulty in this modeling is that electrochemical interfaces involve a solid electrode and a liquid electrolyte. Both materials are usually well treated using different theories. In particular, the electrode generally requires the use of quantum mechanics,” said author Mathieu Salanne. “Our model allows us to perform classical simulations instead, but with a greater precision than what could be done before.”

MetalWalls accounts for the mutual polarization of the electrode and electrolyte, which becomes more important for concentrated electrolytes like ionic liquids. The model and code are freely available.

“We hope that future users will try to tackle new problems that we did not even think of,” said Salanne. “The field of electrochemistry is much wider than the applications we target.”

The researchers are currently exploring complex electrolytes that show enhanced energy storage properties when used in supercapacitors. Accounting for the polarization effects is critical for these ionic liquids, so they hope their simulations will provide accurate descriptions.

Source: “MetalWalls: Simulating electrochemical interfaces between polarizable electrolytes and metallic electrodes,” by Alessandro Coretti, Camille Bacon, Roxanne Berthin, Alessandra Serva, Laura Scalfi, Iurii Chubak, Kateryna Goloviznina, Matthieu Haefele, Abel Marin-Laflèche, Benjamin Rotenberg, Sara Bonella, and Mathieu Salanne, *Journal of Chemical Physics* (2022). The article can be accessed at https://doi.org/10.1063/5.0101777.

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