Better Membranes for Batteries, Fuel Cells & Water Purification

NERSC

Scientific Achievement

Researchers have defined a strategy for architecting porous polymer membranes with well-defined chemical selectivity and efficiency in the molecular scale so objects that can pass through them. Such membranes are key enablers for energy technologies from batteries and fuel cells to water purification and chemical separations. The Berkeley Lab-led team reported their results in the journal Nature.

Significance and Impact

The team demonstrated their synthesis strategy by developing a diverse library of polymer membranes with specific characteristics to promote selective lithium ion transport by creating a well-connected distribution of ion solvation cages. The optimal membrane allows lithium ions – which power rechargeable batteries – to pass with an order of magnitude increase in the flow compared to standard membranes, allowing a battery to deliver more power and to charge more quickly and safely.

Research Details

The team used molecular dynamics simulations run on NERSC's Cori supercomputer to understand how the solvation cages work at a molecular level. These simulations were key to understanding that the cages cause the lithium ions to concentrate more in the new membrane than in those without solvation cages.

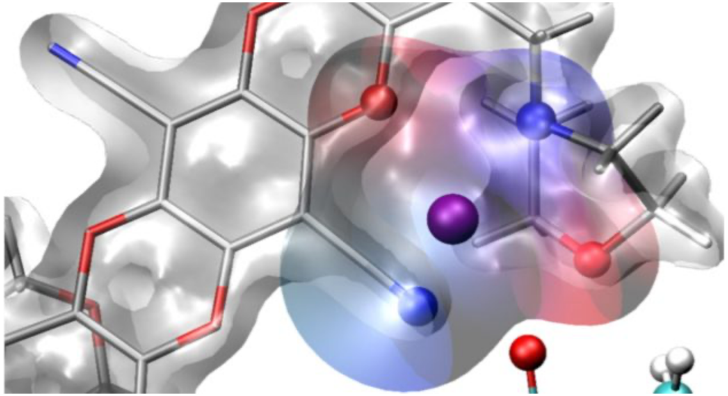

Illustration of caged lithium ions in a new polymer membrane for lithium batteries. Scientists at Berkeley Lab's Molecular Foundry used a drug-discovery toolbox to design the selective membranes. The technology could enable more efficient flows in batteries and energy storage devices. (Credit: Artem Baskin/Berkeley Lab)

Baran, Miranda J.; Carrington, Mark E.; Sahu, Swagat; Baskin,Artem; Song, Junhua; Baird, Michael A.; Han, Kee Sung; Mueller, Karl T.; Teat, Simon J.; Meckler, Stephen M.; Fu,Chengyin; Prendergast, David; Helms, Brett A., "Diversity-oriented synthesis of polymer membranes with ion solvation cages"; NATURE, 592:225+; 2021 APR 8, 10.1038/s41586-021-03377-7

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