Charging ahead with magnesium batteries

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A battery for laptops and smart phones that is long-lasting, safe and affordable is a step closer thanks to work by A*STAR researchers.

Portable electronic devices need smaller batteries with high energy capacities. Now, Man-Fai Ng and colleague Pei Shan Emmeline Yeo, from the A*STAR Institute of High Performance Computing, have investigated a possible cathode material for a magnesium-ion battery to overcome some problems of the common power source, lithium-ion (Li-ion) batteries.

Constraints of Li-ion batteries include low power and limited battery life, which can be significantly improved if lithium is used as the negative electrode or 'anode'.

However, this creates safety issues as during charging and discharging of the battery, microscopic lithium fibers—known as dendrites—can form on the metal anode's surface.

If these dendrites reached the cathode, or positive electrode, the battery can short-circuit and catch fire. "Commercial Li-ion batteries use graphite as the anode to prevent this problem," says Ng. "But the trade-off is that graphite is of lower energy density."

Magnesium metal, on the other hand, does not form dendrites and, in addition to having a higher volumetric energy density than lithium metal, is much more abundant—reducing the cost of raw materials.

Magnesium-ion (Mg-ion) batteries therefore hold promise as next-generation batteries because they would be low cost, safe and have high energy density, explains Ng. One particularly challenge associated with Mg-ion batteries, however, is finding suitable cathode materials.

"Typical Li-ion cathode materials are not compatible with Mg-ion due to its sluggish kinetics of insertion/desertion of magnesium ions in the cathode materials. Therefore, the performance of the Mg-ion batteries is low and of no practical use."

Ng and Yeo used supercomputer modeling to scan for a potential cathode material and identified one-dimensional molybdenum chalcogenide halide nanowires as a promising candidate.

"Among the nanowires studied, the molybdenum selenide nanowire with molecular formula (Mo6Se6) exhibits the best battery performance for its fast ion insertion kinetics and moderately good charge capacity," Ng says.

The team plans to collaborate with experimental groups to verify this theoretical prediction, and continue searching for potential cathode materials for Mg-ion battery using first-principles modeling techniques.

Ng says first-principles modeling is a powerful tool for battery research as it can accurately study the structural and electronic properties of electrode and electrolyte materials; and the interactions between different materials.

More importantly, he says, it can be used for fast screening of materials with desired properties to speed up the search for useful materials to make Mg-ion batteries a reality sooner.

More information: Pei Shan Emmeline Yeo et al. First-Principles

Study of Molybdenum Chalcogenide Halide Nanowires for Mg-Ion Battery Cathode Application, *Chemistry of Materials* (2015). DOI: 10.1021/acs.chemmater.5b01231

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