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Niobium tungsten oxides for high-rate lithium-ion energy storage

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Abstract

The maximum power output and minimum charging time of a lithium-ion battery depend on both ionic and electronic transport. Ionic diffusion within the electrochemically active particles generally represents a fundamental limitation to the rate at which a battery can be charged and discharged. To compensate for the relatively slow solid-state ionic diffusion and to enable high power and rapid charging, the active particles are frequently reduced to nanometre dimensions, to the detriment of volumetric packing density, cost, stability and sustainability. As an alternative to nanoscaling, here we show that two complex niobium tungsten oxides—$Nb_{16}W_5O_{55}$ and $Nb_{18}W_{16}O_{93}$, which adopt crystallographic shear and bronze-like structures, respectively—can intercalate large quantities of lithium at high rates, even when the sizes of the niobium tungsten oxide particles are of the order of micrometres. Measurements of lithium-ion diffusion coefficients in both structures reveal room-temperature values that are several orders of magnitude higher than those in typical electrode materials such as $Li_4Ti_5O_{12}$ and $LiMn_2O_4$. Multielectron redox, buffered volume expansion, topologically frustrated niobium/tungsten polyhedral arrangements and rapid solid-state lithium transport lead to extremely high volumetric capacities and rate performance. Unconventional materials and mechanisms that enable lithiation of micrometre-sized particles in minutes have implications for high-power applications, fast-charging devices, all-solid-state energy storage systems, electrode design and material discovery.

New class of materials could be used to make batteries that charge faster

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Summary: Researchers have identified a group of materials that could be used to make even higher power batteries. The researchers used materials with a complex crystalline structure and found that lithium ions move through them at rates that far exceed those of typical electrode materials, which equates to a much faster-charging battery.

Researchers have identified a group of materials that could be used to make even higher power batteries. The researchers, from the University of Cambridge, used materials with a complex crystalline structure and found that lithium ions move through them at rates that far exceed those of typical electrode materials, which equates to a much faster-charging battery.

Although these materials, known as niobium tungsten oxides, do not result in higher energy densities when used under typical cycling rates, they come into their own for fast charging applications. Additionally, their physical structure and chemical behaviour give researchers a valuable insight into how a safe, super-fast charging battery could be constructed, and suggest that the solution to next-generation batteries may come from unconventional materials. The results are reported in the journal *Nature*.

Many of the technologies we use every day have been getting smaller, faster and cheaper each year -- with the notable exception of batteries. Apart from the possibility of a smartphone which could be fully charged in minutes, the challenges associated with making a better battery are holding back the widespread adoption of two major clean technologies: electric cars and grid-scale storage for solar power.

"We're always looking for materials with high-rate battery performance, which would result in a much faster charge and could also deliver high power output," said Dr Kent Griffith, a postdoctoral researcher in Cambridge's Department of Chemistry and the paper's first author.

In their simplest form, batteries are made of three components: a positive electrode, a negative electrode and an electrolyte. When a battery is charging, lithium ions are extracted from the positive electrode and move through the crystal structure and electrolyte to the negative electrode, where they are stored. The faster this process occurs, the faster the battery can be charged.

In the search for new electrode materials, researchers normally try to make the particles smaller. "The idea is that if you make the distance the lithium ions have to travel shorter, it should give you higher rate performance," said Griffith. "But it's difficult to make a practical battery with nanoparticles: you get a lot more unwanted chemical reactions with the electrolyte, so the battery doesn't last as long, plus it's expensive to make."

"Nanoparticles can be tricky to make, which is why we're searching for materials that inherently have the properties we're looking for even when they are used as comparatively large micron-sized particles. This means that you don't have to go through a complicated process to make them, which keeps costs low," said Professor Clare Grey, also from the Department of Chemistry and the paper's senior author. "Nanoparticles are also challenging to work with on a practical level, as they tend to be quite 'fluffy', so it's difficult to pack them tightly together, which is key for a battery's volumetric energy density."

The niobium tungsten oxides used in the current work have a rigid, open structure that does not trap the inserted lithium, and have larger particle sizes than many other electrode materials. Griffith speculates that the reason these materials have not received attention previously is related to their complex atomic arrangements. However, he suggests that the structural complexity and mixed-metal composition are the very reasons the materials exhibit unique transport properties.

"Many battery materials are based on the same two or three crystal structures, but these niobium tungsten oxides are fundamentally different," said Griffith. The oxides are held open by 'pillars' of oxygen, which enables lithium ions to move through them in three dimensions. "The oxygen pillars, or shear planes, make these materials more rigid than other battery compounds, so that, plus their open structures means that more lithium ions can move through them, and far more quickly."

Using a technique called pulsed field gradient (PFG) nuclear magnetic resonance (NMR) spectroscopy, which is not readily applied to battery electrode materials, the researchers measured the movement of lithium ions through the oxides, and found that they moved at rates several orders of magnitude higher than typical electrode materials.
Most negative electrodes in current lithium-ion batteries are made of graphite, which has a high energy density, but when charged at high rates, tends to form spindly lithium metal fibres known as dendrites, which can create a short-circuit and cause the batteries to catch fire and possibly explode.

"In high-rate applications, safety is a bigger concern than under any other operating circumstances," said Grey. "These materials, and potentially others like them, would definitely be worth looking at for fast-charging applications where you need a