Computer model fills fundamental knowledge gaps of a high performance solar material

June 29 2016

Laboratory-scale solar cells based on inexpensive, crystalline materials called perovskites have emerged as serious contenders to silicon in terms of their efficiency at capturing energy from sunlight. Unfortunately, the neglect of fundamental research into perovskites in favor of close focus on its solar applications has left holes in basic knowledge about the material itself. A*STAR researchers are helping to fill some of these gaps—and by doing so could propel perovskite solar cell performance to the next level.

Methylammonium lead iodide, the quintessential perovskite, consists of a repeating array of lead and iodine atoms bonded to form a cage-like structure—like a nanoscopic, three-dimensional form of chicken wire. Trapped within each tiny cage sits a methylammonium molecule, held in place by hydrogen bonds.

Khuong Ong at A*STAR's Institute of High Performance Computing and his co-workers have been exploring how methylammonium lead iodide's basic properties shift as the material's cage-like structure expands—mimicking the effect of temperature increases. This volume change disrupts the internal network of hydrogen bonds, causing a reorientation of the methylammonium unit within each cage, which in turn affects the perovskite's optical and electrical properties.

Early experimental work had suggested that methylammonium lead

iodide shape-shifts between three distinct structures, or 'phases', as the material expands. But later work suggested that a fourth phase might form under certain conditions. Ong and his team used a model to simulate the structure's response to expansion, from which they could calculate the most stable structure at any given volume. Their results confirm that a fourth phase—which will have its own unique combination of properties, and may turn out to be useful for solar devices—forms at certain intermediate sizes.

"Our study guides the solar cell community to explore conditions for the existence of these different structural phases in methylammonium lead iodide," Ong says. Now that the team has established the structure of this fourth phase, techniques pioneered by the computer chip industry can be used to selectively grow it in the lab, probe its properties and test its performance in solar devices.

Meanwhile, Ong and his team will continue to use computer models to explore the different phases perovskites can form, establish how the material's properties change as a result—and test the potential of structural embellishments to boost sunlight capture: "We are looking for new ways to 'multi functionalize' the perovskite and improve its efficiency as a solar material," Ong says.

More information: Khuong P. Ong et al. Structural Evolution in Methylammonium Lead Iodide CHNHPbI, *The Journal of Physical Chemistry A* (2015). DOI: 10.1021/acs.jpca.5b09884

Provided by Agency for Science, Technology and Research (A*STAR), Singapore