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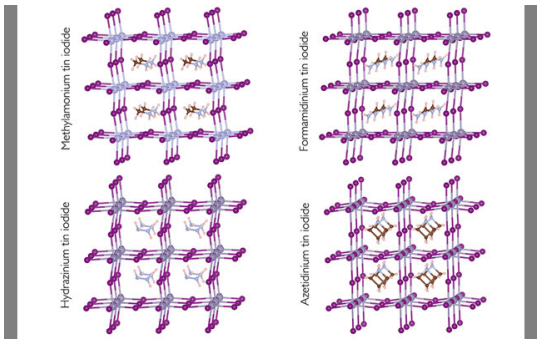
Georgia Tech Engineers Simulate Solar Cell Work Using Supercomputers

Perovskite research shows promise for future inexpensive, efficient solar options

Solar energy has become a popular renewable source of electricity around the world with silicon serving as the primary source due to its efficiency and stability. Because of silicon's relatively high cost, hybrid organic-inorganic perovskites (HOIPs) have emerged as a lower-cost – and highly efficient – option for solar power, according to a recent study by Georgia Institute of Technology (Georgia Tech) researchers.



Four lead-free perovskites were simulated using Comet at the San Diego Supercomputer Center and Stampede2 at the Texas Advanced Computing Center. These simulations show that these materials exhibit promising features for solar energy options. They are now being synthesized for further investigation. Credit: H. Tran et al (Georgia Institute of Technology), V. Ngoc Tuoc (Hanoi University of Science and Technology)

The name perovskite refers not only to a specific mineral ($CaTiO_3$) found in Russia's Ural Mountains, but also to any compound that shares its structure. A search for stable, efficient, and environmentally safe perovskites has created an active avenue in current materials research, with the new Georgia Tech findings relying on simulations done on *Comet* at the San Diego Supercomputer Center (SDSC) and *Stampede2* at the Texas Advanced Computing Center (TACC).

However, the presence of lead in the most promising perovskite candidates, methylammonium and formamidinium lead halides, has raised concerns. Moreover, these materials have shown to be unstable under certain environmental conditions.

The Georgia Tech researchers worked with colleagues at the Hanoi University of Science and Technology in Vietnam to create simulations that identified four lead-free perovskites as promising candidates for solar cell materials. Two of them have already been synthesized and

the other two are recommended for further investigations.

“This research relied on large-scale computations – a first step in our overall plan, which begins with showing simulations of this chemical space of HOIPs,” said Huan Tran, a Georgia Tech materials science and engineering professor and co-author of Lead-free HOIPs for Solar Applications, which was published earlier this year in *The Journal of Chemical Physics*.

Allocations on *Comet* and *Stampede2* were provided via the National Science Foundation’s Extreme Science and Engineering Discovery Environment (XSEDE) program. “Next, we will use these simulations to collaborate with experimental experts who can synthesize and test the predicted HOIPs – no personal computer can handle this level of computations. Hence the XSEDE supercomputers are a critically important aspect of our project.”

Tran and co-author Vu Ngoc Tuoc, a theoretical physics professor at the Hanoi University of Science and Technology, relied heavily upon *Comet* and *Stampede2* for the large-scale computations that allowed them to conduct their research at a much higher level of detail.

They also relied on the SDSC and TACC support staff to help when needed. “The technical support provided by both groups was simply excellent as they helped us solve our problems very efficiently and promptly,” said Tran. “In the coming era of materials informatics, computational materials data is the most important infrastructure, and I find that *Comet*, *Stampede2*, and other XSEDE facilities provide the ideal platform for boosting the development of these areas.”

This research was supported by Vingroup Innovation Foundation under project VINIF.2019.DA03, and XSEDE (TG-DMR170031). The structures of the HOIPs reported in this work are available in the supplementary material and at http://godeepdata.org/.

MEDIA CONTACT

Jan Zverina, 858-534-5111, jzverina@sdsc.edu