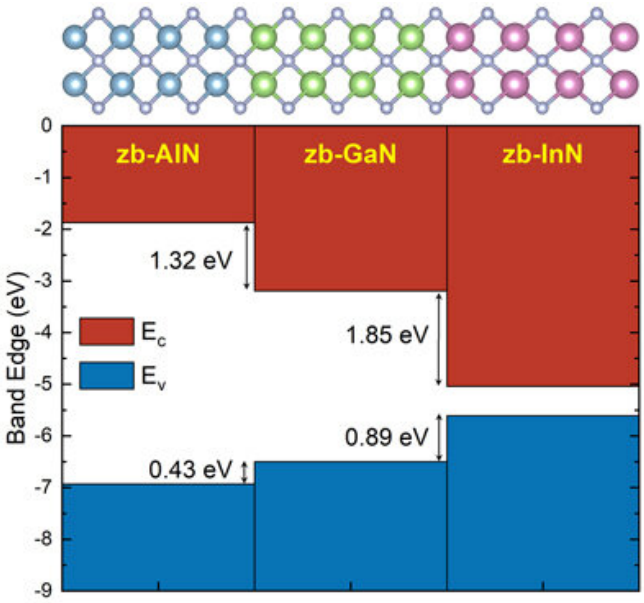
Bright early light of LEDs

July 8 2020, by Jorge Salazar



Scientists are using supercomputers to gain insight on new materials that could make LED lighting even brighter and more affordable. New properties have been found in cubic III-nitrides LED materials useful for next-generation solid-state lighting. Credit: Tsai et. al, ACS Omega 2020, 5, 8, 3917-3923

LED lamps are lighting up the world more and more. Global LED sales in residential lighting have risen from five percent of the market in 2013 to 40 percent in 2018, according to the International Energy Agency, and other sectors mirror these trends. An unmatched energy efficiency and sturdiness have made LED lights popular with consumers.

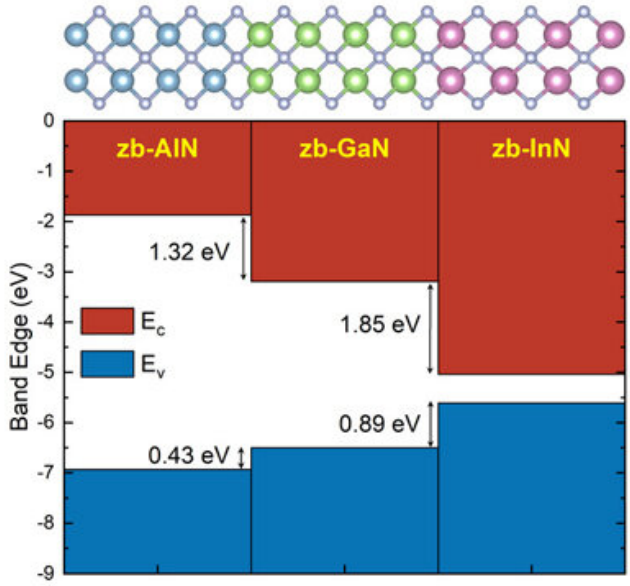
Scientists are currently using supercomputers to gain insight on the crystal structure of new materials that could make LED lighting even brighter and more affordable.

New properties have been found in a promising LED material for next-generation solid-state lighting. A January 2020 study in the chemistry journal *ACS Omega* revealed evidence pointing to a brighter future for cubic III-nitrides in photonic and electronic devices.

"The main finding is that next generation LEDs can, should, and will do better," said study co-author Can Bayram, an assistant professor of electrical and computer engineering at the University of Illinois at Urbana-Champaign. His motivation for studying cubic III-nitrides stems from the fact that today's LED loses much of its efficiency under high injection conditions of current passing through the device, necessary for general lighting.

Bayram's lab builds newly discovered crystals atom by atom in real life as well as in their simulations so that they can correlate experiments with theory. "We need new materials that are scalable to be used for next generation lighting," Bayram said. "Searching for such materials in a timely and precise manner requires immense computational power."

"In this study we are exploring the fundamental properties of cubic-phase aluminium gallium indium nitride materials" Bayram said.



Band gaps and electron affinities of binary and ternary, wurtzite (wz-) and zincblende (zb-) III-nitrides were investigated using a unified hybrid density functional theory, and band offsets between wz- and zb- alloys were calculated using Anderson's electron affinity model. Credit: Tsai et. al, ACS Omega 2020, 5, 8, 3917-3923

"To date, indium gallium nitride-based green LED research has been restricted to naturally-occurring hexagonal-phase devices. Yet they are limited in power, efficiency, speed, and bandwidth, particularly when emitting the green color. This problem fueled our research. We found that cubic phase materials reduce the necessary indium content for the green color emission by ten percent because of a lower bandgap. Also, they quadruple radiative recombination dynamics by virtue of their zero polarization." study co-author and graduate student Yi-Chia Tsai added.

Bayram describes the computational model used as "experimentally-corroborated." "The computed fundamental material properties are so accurate that computational findings have almost one-on-one match with

the experimental ones," he said.

He explained that it's challenging to model compound semiconductors such as gallium nitride because they are compound, unlike elemental semiconductors such as silicon or germanium. Modeling alloys of the compound semiconductors, such as aluminum gallium nitride, are further challenging because, as the saying goes, it's all about location, location, location. Relative atomic positions matter.

"In a unit cell sketch of a crystallography class, Al and Ga atoms are interchangeable. But not so in our computational research," Bayram explained. That's because each atom and its relative position matter when you are simulating the unit cell, a small volume of the entire semiconductor material.

"We simulate the unit cell to save computational resources and use proper boundary conditions to infer the entire material properties. Thus, we had to simulate all possible unit cell combinations and infer accordingly—this approach gave the best computational matching to the experimental ones," Bayram said. Using this approach, they further explored new though not experimentally-realized materials.

To overcome the computational challenges, Bayram and Tsai applied for and were awarded supercomputer allocations by the Extreme Science and Engineering Discovery Environment (XSEDE). XSEDE is a single virtual system funded by the National Science Foundation that scientists can use to interactively share computing resources, data, and expertise. XSEDE-allocated Stampede2 and Ranch systems at the Texas Advanced Computing Center supported Bayram's simulations and data storage.

The Stampede2 supercomputer at the Texas Advanced Computing Center is an allocated resource of the Extreme Science and Engineering Discovery Environment (XSEDE) funded by the National Science Foundation (NSF). Credit: TACC

"XSEDE is a unique resource. We primarily use the state-of-the-art XSEDE hardware to enable material computations. First, I want to stress that XSEDE is an enabler. Without XSEDE, we could not perform this research. We started with Startup then Research allocation grants. XSEDE—over the last two years—provided us with Research allocations valued at nearly $20,000 as well. Once implemented, the outcome of our research will save billions of dollars annually in energy savings alone," Bayram said.

Bayram stressed that non-scientists can benefit from this basic research into prototype LED materials. "We all need lighting, now more than ever. We not only need lighting for seeing. We need it for horticulture. We need it for communication. We need it for medicine. One percent efficiency increase in general lighting will save us $6 billion annually. In financial terms alone, this is a million times return on investment," he said.

For any semiconductor device, scientists strive to understand the impurities within. The next stage in Bayram's research is to understand how impurities impact new materials and to explore how to dope the new material effectively. Through searching the most promising periodic table groups, he said they're looking for the best elemental dopants, which will eventually help the experimental realization of devices immensely.

Said Bayram: "Supercomputers are super-multipliers. They super-multiply fundamental research into mainstream industry. One measure of success comes when the research outcome promises a unique solution. A one-time investment of $20K into our computational quest will at least lead to $6 billion in savings annually. If not, meaning that the research outcome eliminates this material for further investigation, this early investment will help the industry save millions of dollars and research-hours. Our initial findings are quite promising, and regardless of the outcome the research will ultimately benefit society."

The study, "Band Alignments of Ternary Wurtzite and Zincblende III-Nitrides Investigated by Hybrid Density Functional Theory," was published in the journal *ACS Omega* on January 30, 2020. The study co-authors are Yi-Chia Tsai and Can Bayram, Department of Electrical and Computer Engineering, University of Illinois at Urbana-Champaign. This work is supported by the National Science Foundation Faculty Early Career Development (CAREER) Program under award number

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More information: Yi-Chia Tsai et al. Band Alignments of Ternary Wurtzite and Zincblende III-Nitrides Investigated by Hybrid Density Functional Theory, *ACS Omega* (2020). DOI: 10.1021/acsomega.9b03353

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