Improving LED efficiency through InN nanostructures

Bridging the green gap by using quantum confinement.

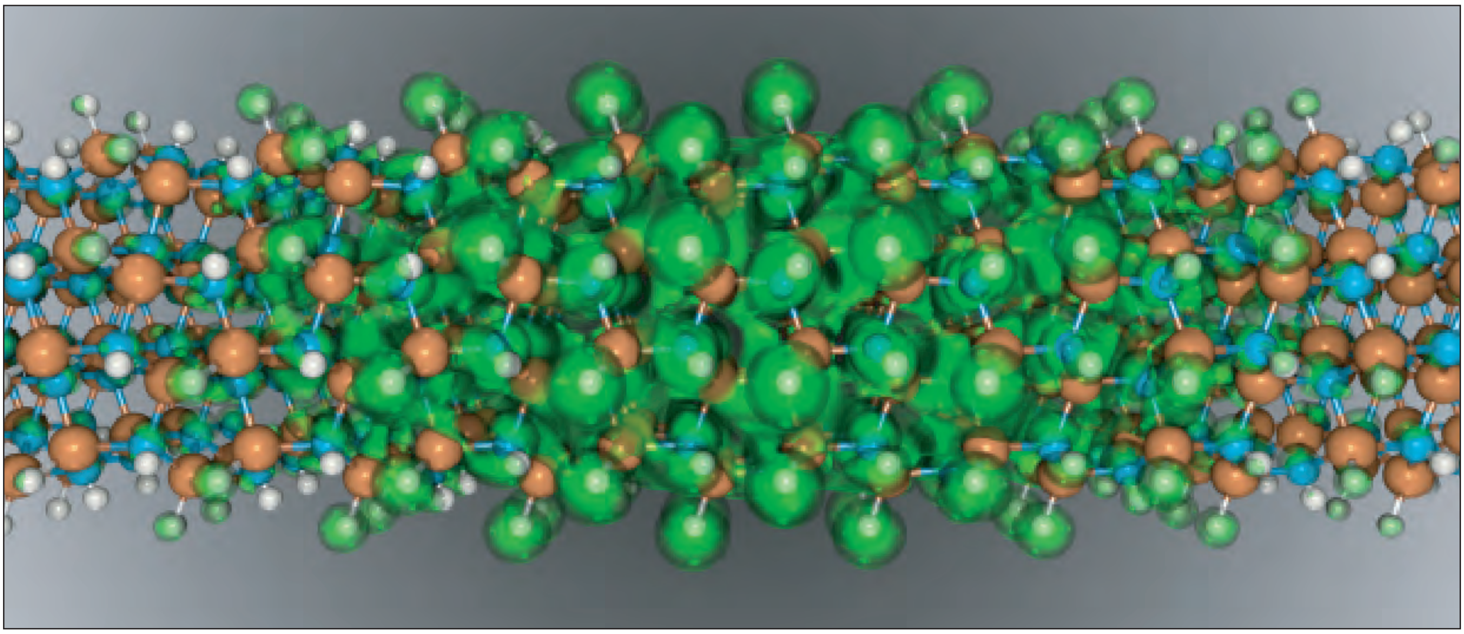
The US Department of Energy's National Energy Research Scientific Computing Center (NERSC) has conducted simulations showing that nanostructures half the width of a DNA strand could enhance the efficiency of LEDs. In particular, efficiency improvements were notable in the 'green gap' portion of the spectrum where efficiency in traditional LED is known to fall (Dylan Bayerl and Emmanouil Kioupakis 'Visible-Wavelength Polarized Light Emission with Small-Diameter InN Nanowires', published online on 14 February 2014, DOI: 10.1021/nl404414r; to be featured in the July issue of Nano Letters).

Using NERSC's Cray XC30 supercomputer 'Edison', Dylan Bayerl and Emmanouil Kioupakis in the University of Michigan's Department of Materials Science and Engineering found that indium nitride (InN), which typically emits infrared light, will emit green light if reduced to 1nm-wide wires. Moreover, just by varying their sizes, the nanostructures could be tailored to emit different colors of light, which could lead to more natural-looking white lighting while avoiding some of the efficiency loss that existing LEDs experience at high power. "Our work suggests that indium nitride at the few-nanometre size range offers a promising approach to engineering efficient, visible light emission at tailored wavelengths," says Kioupakis.

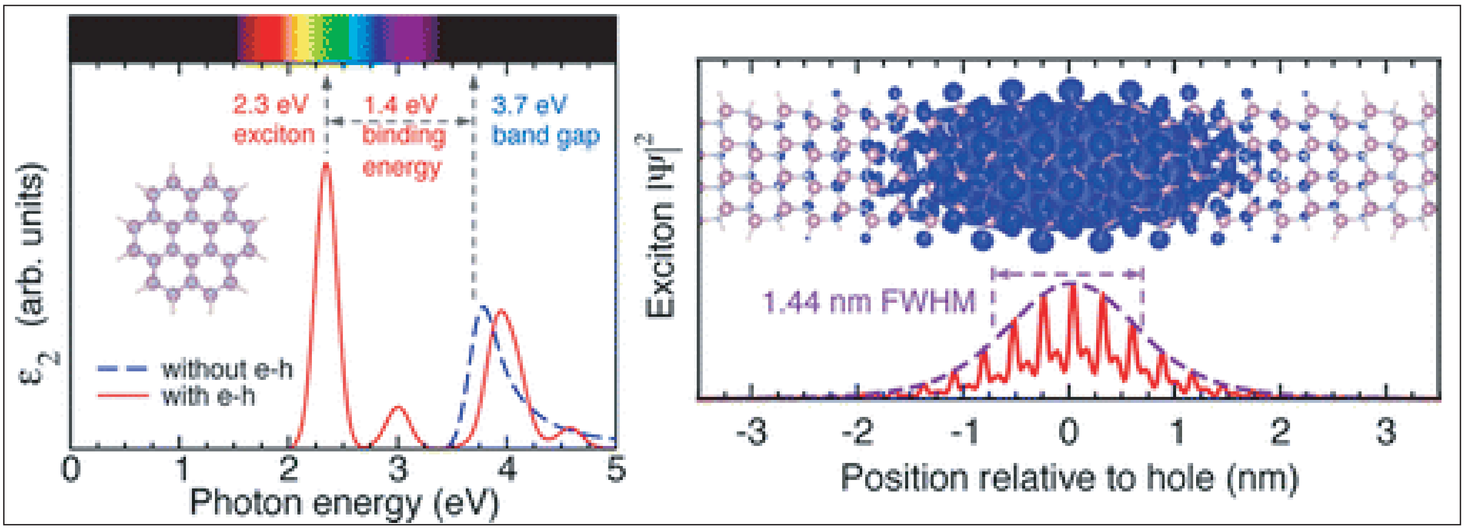
In existing multi-layered LED chips, the outer layers are doped with elements that create an abundance of electrons on one layer and too few (i.e. 'holes') on the other. When the chip is energized, the electrons and holes are pushed together, confined to the intermediate quantum-well layer where they are attracted to combine, shedding their excess energy (ideally) by emitting a photon.

At low power, nitride-based LEDs (most commonly used in white lighting) are efficient, converting most of their energy into light. But when the power is turned up to levels that could light up a room, the efficiency plummets. This 'efficiency droop' effect is especially pronounced in green LEDs, giving rise to the 'green gap'. Nanomaterials offer the prospect of LEDs that can be grown in arrays of nanowires, dots or crystals. The resulting LEDs could not only be thin, flexible and high-resolution, but efficient as well.

"If you reduce the dimensions of a material to be about as wide as the atoms that make it up, then you get quantum confinement. The electrons are squeezed into a small region of space, increasing the bandgap [the energy difference between electrons and holes]," Kioupakis notes. The photons emitted when electrons



This simulation of a 1nm-wide InN wire shows the distribution of an electron around a positively charged hole. Strong quantum confinement in these small nanostructures enables efficient light emission at visible wavelengths. (Visualization: Burlen Loring, Lawrence Berkeley National Laboratory)



Quantum confinement in 1nm-wide InN nanowires shifts optical emission to the visible range at green/cyan wavelengths and inverts the order of the top valence bands, leading to linearly polarized visible-light emission. It also leads to large exciton binding energies of 1.4eV and electronic band gaps in excess of 3.7eV.

and holes combine are hence more energetic. Since the bandgap determines the wavelength of the emitted light (and the wider the bandgap, the shorter the wavelength of light), quantum confinement hence produces shorter-wavelength light.

The bandgap energy for bulk InN is quite narrow (just 0.6eV), so it produces infrared light. In Bayerl and Kioupakis simulated InN nanostructures, the calculated bandgap increased, leading to the prediction that green light would be produced with an energy of 2.3eV. "If we can get green light by squeezing the electrons in this wire down to 1nm, then we can get other colours by tailoring the width of the wire," says Kioupakis. A wider wire should yield yellow, orange or red. A narrower wire, indigo or violet," he adds.

This bodes well for creating more natural-looking light from LEDs. By mixing red, green and blue LEDs, engineers can fine tune white light to warmer, more pleasing hues. The 'direct' method is not practical currently, because green LEDs are not as efficient as their blue and red counterparts. Instead, most existing white lighting comes from blue LED light passed through a phosphor (a solution similar to fluorescent lighting, and not much more efficient). Direct LED lights would not only be more efficient, but the colour of light they produce could be dynamically tuned to suit the time of day or the task at hand.

Using pure InN, rather than layers of alloy nitride materials, would eliminate one factor that contributes to the inefficiency of green LEDs: nanoscale composition fluctuations in the alloys. These have been shown to impact LED efficiency.

Also, using nanowires to make LEDs eliminates the problem of lattice mismatch between layers of different material in layered devices. "When the two materials do not have the same spacing between their atoms and you grow one over the other, it strains the structure, which moves the holes and electrons further apart, making them less likely to recombine and emit light," says Kioupakis. "In a nanowire made of a single material, you do not have this mismatch and so you can get better efficiency," he adds.

The researchers also suspect that the nanowire's strong quantum confinement contributes to efficiency by squeezing the holes and electrons closer together (a subject for future research). "Bringing the electrons and holes closer together in the nanostructure increases their mutual attraction and increases the probability that they will recombine and emit light," Kioupakis says.

While this result points the way towards a promising avenue of exploration, the researchers emphasize that such small nanowires are difficult to synthesise. However, they suspect that their findings can be generalized to other types of nanostructures, such as embedded InN nanocrystals, which have already been synthesised in the few-nanometres range.

NERSC's newest flagship supercomputer 'Edison' was instrumental in the research, says Bayerl. The system's thousands of compute cores and high memory-per-node allowed Bayerl to perform massively parallel calculations with many terabytes of data stored in RAM, making the InN nanowire simulation feasible. "We also benefited greatly from the expert support of NERSC staff," notes Bayerl. Burlen Loring of NERSC's Analytics Group created visualizations for the study. The researchers also used the open-source BerkeleyGW code, developed by NERSC's Jack Deslippe.

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