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Investigating the influence of strain on perovskite lattices

Research Objectives

Dr Xianghua Wang researches strain in relation to perovskite lattices.

Detail

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Bio
Xianghua Wang is an associate professor at Hefei University of Technology. His research is currently focused on light-emitting materials, thin-film processing, and device fabrication featuring low-cost and broad-area processability. He also has research and engineering experience of integrated circuit manufacturing, laser micromachining, and inkjet printing.

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Collaborators
Sichuan Research Center of New Materials, Institute of Chemical Materials, China Academy of Engineering Physics

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Personal Response

What real-world perovskite applications could benefit from your discoveries?

" Lead halide perovskite greatly promotes our understanding of strain effects at the molecular scale, however the toxicity of lead atoms is problematic in practical application. Fortunately, research on strain effects opens the door for tuning semiconductor properties via a strategy other than chemical composition, which adds to our confidence to address the toxicity problem by substituting lead with environment-friendly chemicals. "

Investigating the influence of strain on perovskite lattices

Perovskites are already being closely studied for their advanced material properties – particularly regarding the intriguing ways that they interact with light. Dr Xianghua Wang at Hefei University of Technology in China shows how these properties could be advanced even further, by considering how perovskite lattices are put under strain by the formation of molecular cross-links. By drawing from his discoveries, researchers could gain far greater control over the light emissions of perovskites – potentially expanding their applications in a diverse array of cutting-edge technologies.

Strain is an immensely important quantity for engineers: telling them how much a material will mechanically deform when an external load is applied to it. By measuring the strains of different materials, engineers can then assess how well they are suited for building structures including trains, robots, and skyscrapers.

On molecular scales, the influence of strain manifests itself very differently, but is no less important for researchers to consider. When the orderly molecular lattice of a solid material comes under strain, the inter-atomic bonds which hold it together will be distorted – altering the spatial arrangements of its constituent atoms and molecules. These transformations can have profound effects on the physical properties of these structures.

By fine-tuning the characteristics of the strain applied to these materials to optimise their molecular arrangements, researchers have now realised they can enhance their performance in a wide variety of useful applications. This can also enable researchers to grow molecular lattices on the surfaces of different types of crystal: a technique named 'heteroepitaxy.'

MYSTERIES IN PAST DISCOVERIES

Wang and colleagues have explored the synthesis of lead sulphide nanoparticles using thiol functional trimethoxy silane. As they discovered, this process can be improved by the network of alternating chains of silicon and oxygen atoms, named 'siloxane.' Here, siloxane molecules were derived from the trimethoxy silane by reaction with a trace of water in the solvent and used as 'ligands', bound through the thiol group to a metal atom. By applying siloxane ligands, the researchers could ensure that the lead and sulphur atoms in the solution would cluster into nanoparticles with more uniform sizes – enhancing their light-absorbing properties.

Perovskite crystals.

Photo Credit: Rob Lavinsky, iRocks.com – CC-BY-SA-3.0, CC BY-SA 3.0, via Wikimedia Commons

In each of these cases, Wang suspected that the molecular behaviours he observed were influenced by strain modulation. However, since this property was intertwined with several other, unrelated effects, quantifying the influence of strain modulation on its own presented a difficult challenge. To overcome this problem, Wang has now shifted his focus to study a new class of materials named 'perovskites.'

GROWING UNIFORM NANOCRYSTALS

Featuring unique arrangements of atoms and molecules in their lattices, perovskites are now well known among materials physicists for their unique light-emitting and absorbing properties. In particular, they are already being intensively studied for their promising potential in solar cell technology – which aims to convert sunlight into electrical power as efficiently as possible. Yet for Wang, these properties presented an ideal platform for investigating the effects of strain modulation on molecular-scale structures.

Through his latest studies, Wang has revisited this previous line of research, by investigating the influence of strain modulation on a process named 'passivation'. Here, materials are treated with a molecular coating which may render solution processability and deactivate surface trap states – reducing unwanted effects such as corrosion and nonradiative recombination. In this case, nanocrystals of the perovskite $CsPbBr_3$ were synthesised by injecting the precursor of siloxane ligands into a dispersion of the perovskite nanocrystals.

Wang's team used a combination of techniques to study the resulting molecular structure in close detail, including 'Fourier-transform infrared spectroscopy' – which identifies the structure via vibrational characteristics. In addition, they used 'X-ray photoelectron spectroscopy' to measure the elemental composition on the surface of the sample. With this combined approach, the researchers discovered that the perovskite's passivation with siloxane ligands was strongly influenced by covalent bonds between sulphur atoms in the siloxane, and lead atoms in the perovskite. The result was modulated by a cross-linked network of siloxane molecules – introducing strain to the solid perovskite lattice. With this approach, the team could grow perovskite nanocrystals which were mostly uniform in size – just as Wang had observed in his previous experiments.

The team used Fourier-transform infrared spectroscopy to assess vibrational characteristics.

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Quantum dots allow researchers to carefully control the properties of their photoluminescence.

BOOSTING PHOTOLUMINESCENCE EFFICIENCY

One further effect observed in these recent studies is that strain in the lattice of colloidal particles also occurred perpendicular to its surface, making it easy to identify. Wang had already observed the consequences of this effect by measuring the out-of-plane lattice spacings for colloidal zinc oxide films on silica substrates.

Through further analysis, the researchers showed that this effect can provide a boost to a perovskite's 'photoluminescence'. This effect arises when an electron contained in an atom is excited to a higher energy level, after absorbing a photon with just the right wavelength. After this initial excitation, electrons will relax back to their original energy levels over a wide range of timescales, re-emitting a photon in the process. In turn, photoluminescence can enable materials to glow, even when they are no longer being illuminated.

Perovskites are already well known for their high photoluminescence efficiencies, which allow them to emit much of the light they originally absorb. Yet when subject to optimised strain patterns induced by siloxane ligands, as Wang's team have shown, this efficiency can be boosted even further – potentially reaching as high as 99%.

By fine-tuning the chemical composition of perovskite lattice, ligand type and density on the surface, the results also reveal that the wavelengths of re-emitted photons can be carefully controlled. This discovery could lead to exciting new capabilities in colour conversion – where nanocrystals illuminated with blue light can re-emit these photons as pure green light – or potentially even longer wavelengths.

MONOLAYER THICKNESS

The final important outcome of Wang's latest experiments is that passivation with siloxane ligands remains effective, even when ligands on the nanocrystals formed are just a single molecule thick. The property presents promising opportunities for future designs of advanced new nanomaterials, and could also enhance the efficiency of 'electroluminescence' – where materials emit light in response to passing electric currents and fields.

In turn, the team's discoveries could pave the way for a diverse array of applications in 'optoelectronics' – in which electronic devices are used to detect and control light. These devices are based on the quantum processes which occur when light interacts with electronic materials, especially semiconductors, whose electrical properties lie in between those of conductors and insulators.

Perhaps the most important implications for this research will be for structures named 'quantum dots': semiconductor nanoparticles just a few nanometres in size, which behave much like individual artificial atoms. When illuminated with ultraviolet light, photoluminescence causes a single quantum dot electron to be excited to a higher energy level, before relaxing and re-emitting a photon.

In this case, the wavelength of this photon depends precisely on the difference in the excitonic energy levels between the excited state and the ground state. This difference in turn depends on the band gap, confinement energy, and exciton binding energy that is affected by factors including the nanoparticle's size, shape, composition, and structure.

As a result, quantum dots allow researchers to carefully control the properties of their photoluminescence. Such advanced properties mean that their potential use is now being carefully explored in a diverse array of cutting-edge devices: including lasers, solar cells, and quantum computers.

CHARACTERISING STRAIN FIELDS

Wang and his colleagues hope that their future goals could be achieved by designing new 'processing kits', which can characterise these strain fields in normal lab conditions. Ultimately, their research now offers enormous potential for various highly exciting future discoveries, which could one day prove to transform our ability to capture and control light.

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