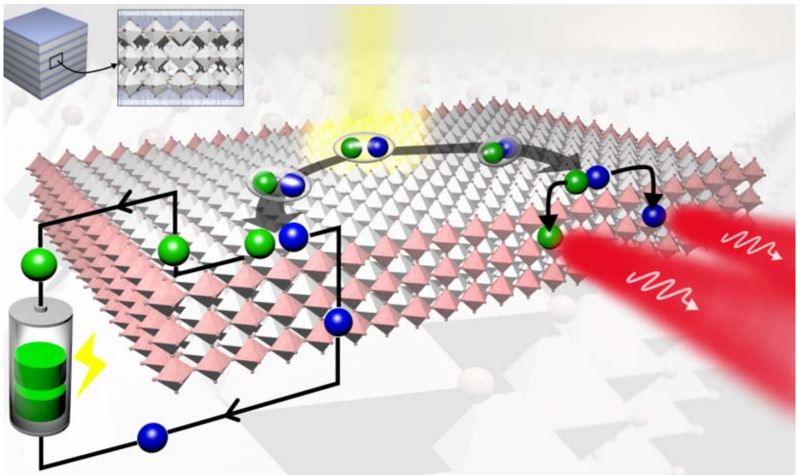
Perovskite edges can be tuned for optoelectronic performance

March 9, 2017



How it works, from sunshine (yellow beam) to LED light and photovoltaics -- Edge-states at the edges of the 2D perovskite layers lead to dissociation of electron-hole pairs (excitons) to free carriers for efficient photovoltaics of more than 12 percent (left). Dissociated carriers captured and located at the edge-states live longer while being protected from loss mechanisms (right), which results in efficient fluorescence of a few tens of percent applicable to next-generation LEDs. (top) Material structure sketching the stacking of nanometer-thick layers of 2D perovskite and organic spacing layers. Credit: Los Alamos National Laboratory

In the eternal search for next generation high-efficiency solar cells and LEDs, scientists at Los Alamos National Laboratory and their partners are creating innovative 2D layered hybrid perovskites that allow greater freedom in designing and fabricating efficient optoelectronic devices. Industrial and consumer applications could include low cost solar cells, LEDs, laser diodes, detectors, and other nano-optoelectronic devices.

"Our material is a layered compound, meaning it is a stack of 2D layers of perovskites with nanometer thickness (like a stack of sheets), and the 2D perovskite layers are separated by thin organic layers," said Jean-Christophe Blancon, lead author on a paper out today in the journal *Science*'s First Release distribution. "This work could overturn conventional wisdom on the limitations of device designs based on layered perovskites."

The 2D, near-single-crystalline "Ruddlesden-Popper" thin films have an out-of-plane orientation so that uninhibited charge transport occurs through

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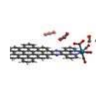

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The team investigated both photophysical and optoelectronic properties of phase-pure homogenous 2D perovskites. They were able to show that thin films have an intrinsic mechanism for dissociation of the strongly bound electron-hole pairs (excitons) to long-lived free-carriers provided by lower energy states at the edges of the layered perovskites.

Moreover, once carriers are trapped in these edge states, they remain protected and do not lose their energy via non-radiative processes. They can contribute to photocurrent in a photovoltaic (PV) device or radiatively recombine efficiently for light-emission applications. "These materials are quantum hybrid materials, possessing physical properties of both organic semiconductors and inorganic semiconducting quantum wells. We are just beginning to understand the interplay of the organic and inorganic components in 2D perovskites and this result underpins how unique properties can arise from competing physical properties," said Jared Crochet of the Physical Chemistry and Applied Spectroscopy group at Los Alamos.

"These results address a long-standing problem not just for the perovskite family, but relevant to a large group of materials where edges and surface states generally degrade the optoelectronic properties, which can now be chemically designed and engineered to achieve efficient flow of charge and energy leading to high-efficiency optoelectronic devices," said Aditya Mohite, who leads the perovskite program in the Material Synthesis and Integrated devices group at Los Alamos.

"The 2D hybrid perovskites continue to surprise. When we first designed these materials we were hoping that high quality samples of them would exhibit novel optoelectronic properties," said co-author Mercouri Kanatzidis of Northwestern University. "Well, they have done so and then some. They have exceeded our expectations and are proving to be truly amazing systems. We have only scratched the surface of what is there—sorry for the pun—in this 2D family and we anticipate continued excitement going forward."

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More information: "Extremely efficient internal exciton dissociation through edge states in layered 2-D perovskites," *Science* 09 Mar 2017: **DOI: 10.1126/science.aal4211**

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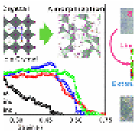

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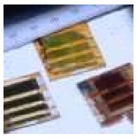

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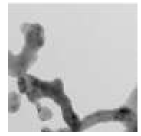

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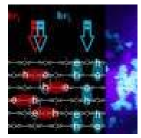

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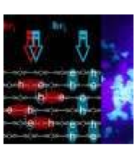

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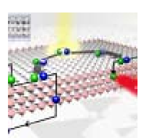

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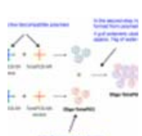

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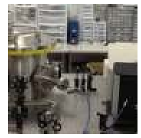

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