Lanthanum chromium oxide's energetic dance with light

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Scientists at Pacific Northwest National Laboratory, University College London, and Florida International University have determined how a particular oxide material, lanthanum chromium oxide (LCO), interacts with visible and ultraviolet light.

The absorption of light by certain kinds of materials results in conversion of light energy into electrical energy, a process of great importance in energy technology. The sun is abundant in visible light that looks green to the eye, and being able to convert sunlight into electricity leads to a free, clean energy source that leaves no carbon footprint. Such energy sources are essential to a safe, secure, and environmentally friendly energy future, something that should be of interest to every American.

Only certain kinds of materials can absorb light and convert the light into electricity. These materials are called semiconductors. "Semi" is a Latin prefix meaning "half." So, a semiconductor can be thought of as a half or partial conductor of electricity, relative to metals, which are excellent conductors of electricity. The reason that a semiconductor is only a partial conductor of electricity is because its energy bands, or orbitals, where electrons reside, are separated into two kinds. One is called the valence band (VB). Electrons in the VB are not mobile and, therefore, cannot conduct electricity. The other is called the conduction band (CB), and electrons in the CB are mobile. In semiconductors, the concentration of electrons in the CB is low compared to that in metals, resulting in partial conduction. The VB and CB are separated by a fixed quantity of energy, called the band gap. If a semiconductor is irradiated with light whose energy is greater than the band gap, electrons can absorb the light and be lifted from the VB to the CB, resulting in light-induced electrical conductivity. Finding ways to modify the properties of semiconductors so that they absorb light in particular energy ranges is very important in photovoltaics, the science of light-to-electricity energy conversion.

Materials that are of current interest in photovoltaics often include atoms that are toxic or rare. These include gallium, arsenic, cadmium and tellurium. Moreover, the surfaces of these photovoltaic materials react with oxygen in the atmosphere and form oxides, which changes their properties in ways that make them less useful for photovoltaic technologies. An ideal class of materials for future photovoltaic applications is the metal oxides, specifically complex metal oxides. These materials can be made from abundant, inexpensive atoms, and are stable in air because they are already oxides. However, the optical properties of most complex oxides are themselves rather complex, and very poorly understood. Gaining a detailed understanding of one such oxide, LCO, is the focus of this study.

The team's approach was to make ultra-pure LCO by depositing separate beams of lanthanum, chromium, and oxygen atoms onto a solid substrate, using a process called molecular beam epitaxy. They then shined light on the LCO film and varied the energy of the light, spanning the visible and near ultraviolet portions of the electromagnetic spectrum. They determined the energies at which the light was absorbed by the LCO. The light absorption spectrum is quite complex, and it is not possible to understand the origin of the different absorption peaks without the help of theoretical calculations. To this end, the team carried out a detailed set of theoretical calculations in which they simulated the light absorption process in LCO for different light energies. Doing so allowed them to determine in detail what parts of the CB and VB in LCO were involved in specific absorption events. What they learned was quite surprising. Earlier experimental investigations led to the conclusion that the onset of electrical conductivity occurs for a light energy of ~3.3 electron volts. The team's combined experimental and theoretical investigation showed that the onset of electrical conductivity actually occurs for a much higher light energy, ~4.8 electron volts. The absorption features at lower energies (such as 3.3 electron volts) are actually due to localized excitations that do not result in electricity being conducted across the LCO, and were misinterpreted in earlier studies.

This investigation is part of larger study aimed at shifting the band gap of LCO to lower values, where the sun is more abundant in sunlight. The team's strategy is to replace some of the lanthanum atoms in the LCO with strontium atoms. In the limit of 100% replacement of lanthanum with strontium, we get strontium chromium oxide, which is a metal. The preliminary results indicate that as the percentage of lanthanum replaced with strontium increases, the band gap does indeed decrease into the desired range. This result, if found to be reproducible, means that strontium lanthanum chromium oxide is an attractive candidate for a tunable band gap oxide semiconductor that would be useful for photovoltaic, or "light-harvesting" technology.

More information: Sushko, P. et al. Multiband Optical Absorption Controlled by Lattice Strain in Thin-Film LaCrO3. *Physical Review Letters* 110(7):077401. DOI: 10.1103/PhysRevLett.110.077401

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