Researchers decipher the dynamics of electrons in perovskite crystals

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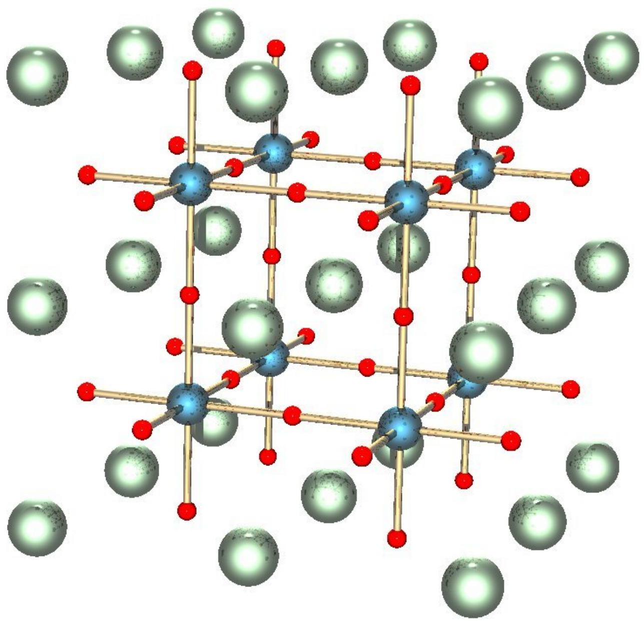

This is a POV ray drawing of a small section of the lattice of an imaginary perovskite. The red atoms are oxygen anions while the the green atom represents the larger cation, and the blue central atom the smaller cation, typically with a higher oxidization state. I created this file by writing a XYZ file using a spreadsheet after reading cotton and wilkinson, this was edited using the text editor of ORTEP. ORTEP was used to write the pov file, then POVray was used to draw it. Credit: Wikimedia Commons.

Physicists at Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) have proven that incoming light causes the electrons in warm perovskites to rotate, thus influencing the direction of the flow of electrical current. They have thus found the key to an important characteristic of these crystals, which could play an important role in the development of new solar cells. The results have now been published in *Proceedings of the National Academy of Sciences*.

The sun is an important source of renewable energy. Its radiation energy provides heat, and sunlight can be converted into electricity thanks to photovoltaics. Perovskites, crystalline compounds that can be simply manufactured using chemical processes, are considered a promising material for photovoltaics. Under laboratory conditions, prototypes have achieved surprising levels of efficiency.

There is little knowledge about precisely why perovskites are so powerful. "Two factors are decisive for generating electrical energy cost-efficiently from sunlight," says Dr. Daniel Niesner from the Chair of Solid State Physics at FAU. "On the one hand, the light must excite as many electrons as possible in a layer that's as thin as possible. On the other, the electrons must be able to flow as freely as possible to the electrodes that pick up the current."

Researchers suspect that perovskites make particularly good use of the rotation of electrons for efficient current flow. "Each electron has spin, similar to the intrinsic rotation of a billiard ball," explains Niesner. "As is the case with billiard balls, where left-hand or right-hand spin when they are hit with the cue leads to a curved path on the table, scientists have suspected that rotation and forward movement in electrons in perovskites could also be linked."

Orderly atomic structure

Physicists at FAU in Erlangen have now confirmed this suspicion for the first time. In their experiments, they used a laser whose light also has spin or a direction of rotation. The result: If a crystal is exposed to light with a left-hand spin, the electrons move to the left. If the direction of the light is reversed, the direction of the flow of electrons also reverses. "The experiments clearly demonstrate that the direction of rotation of the electrons and the direction of flow of current are linked."

Until now, scientists presumed that the atomic structure of perovskites was too 'orderly' for such behaviour. In actual fact, experiments with cooled perovskite crystals show only a very weak link between the direction of rotation of the electrons and the direction of current flow. "This changes, however, when the crystals are heated to room temperature because the movement of the atoms leads to fluctuating deviations of the highly-ordered structure," says Nieser. "The heat enables the crystals of perovskite to link the direction of rotation and flow of the electrons. A 'normal' crystal couldn't do that."

The discovery of the connection between heat and spin in electrons means that the FAU researchers have uncovered a vital aspect of the unusual flow of current in perovskites. Their work could contribute to improving the understanding of the high energy efficiency of these crystals and to developing new materials for photovoltaics in the future.

More information: Daniel Niesner et al, Structural fluctuations cause spin-split states in tetragonal (CH3NH3)PbI3 as evidenced by the circular photogalvanic effect, *Proceedings of the National Academy of Sciences* (2018). DOI: 10.1073/pnas.1805422115

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