Transparent electronics research gains momentum

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Transparent electronics are the future, according to researchers including José A. Flores-Livas and Miglė Graužinytė from the research group headed by Stefan Goedecker, Professor of Computational Physics at the University of Basel. However, the relevant technological development is progressing sluggishly due to a shortage of certain transparent semiconductors with a high level of conductivity.

Impurities for optimisation

The electronic or optical properties of semiconductors can be manipulated and optimised by making use of appropriate impurities in the material. This doping with impurities, for example in transistors, changes the charge carrier density, thus increasing conductivity.

Identifying suitable impurities in the periodic table, however, often involves years of expensive laboratory experimentation. Researchers are attempting to speed up this process by using computer simulations. They use these to calculate the most promising candidates on the basis of physical laws that describe the interaction between the impurity and the material of the conductor. Potential candidates can then be tested in the laboratory in a targeted manner.

Shortage of special high-performance conductors

Researchers at the University of Basel used the Piz Daint supercomputer to carry out such complex simulations with the aim of finding suitable impurities that can be used to produce transparent conductors. But when it comes to transparent conductors, the main shortage is of high-performance conductors known as P-Type (positively charged carriers) in which the implanted impurity has one electron too few. Conversely, conductors known as N-Type (negatively charged carriers) are doped with elements that have, so to speak, a spare electron.

According to the researchers, it was recently found that the environmentally friendly and earth-abundant tin monoxide could be a very promising material for the production of transparent and high-performance P-Type conductors. It is also suitable for what is known as ambipolar doping, which is when both negative and positive charge carriers are combined in bipolar conductors. However, until now only a handful of elements have been examined that could be suitable as impurities for equipping the tin monoxide-based semiconductor with the desired properties.

Promising alkali metals

Through their computations, the researchers identified alkali metals as full of potential. They were able to identify five alkali metals (lithium, sodium, potassium, rubidium and caesium) that could be introduced into tin monoxide in order to enable high-performance and transparent P-Type semiconductors. In addition, according to the researchers, the computations established 13 elements suitable for doping with N-Type charge carriers in tin monoxide. "If these elements can be successfully introduced into tin monoxide and the desired semiconductor can be produced, this would open new avenues for a range of transparent technologies," says Flores-Livas.

More information: Miglė Graužinytė et al. Towards bipolar tin monoxide: Revealing unexplored dopants, *Physical Review Materials*

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