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NEW CLASS OF QUANTUM MATERIALS FOR CLEAN ENERGY TECHNOLOGY

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Researchers from IIT Bombay have discovered special properties in a class of materials called “semi-Dirac metals” that have been recently talked about in the scientific literature. Examples of semi-Dirac metals are systems such as TiO2/V2O3 nanostructures. Through calculations, the researchers have shown that such materials would be transparent to light of a given frequency and polarisation when it is incident along a particular direction. The material would be opaque to the same light when it falls on it from a different direction. There are many known applications for transparent conducting films – the common example being touch screens used in mobiles. These results were published in *Physical Review B.*

“Our results in this paper show a very high optical conductivity of semi-Dirac materials for electromagnetic waves [light waves] of a specific frequency and specific polarisation” says Alestin Mawrie, a post-doctoral fellow at Department of Electrical Engineering, and the first author of the paper. Optical conductivity is a measure of the opacity offered by the material to the passage of light through it.

Normal metals like gold and silver are good conductors of electricity. A key aspect that decides the quality of conduction is the way energy depends on the momentum of electrons. Dirac metals differ from normal metals in that the energy depends linearly on the momentum. This difference is responsible for their unique properties. Semi-Dirac metals behave like Dirac metals in one direction and like normal metals in the perpendicular directions (since their microscopic structure is different along the two directions).

Within any material, charge carriers, such as electrons, acquire an effective mass which is different from their bare mass depending on the nature of the material. The effective mass and the number of states available for the electron to occupy when it is excited by an electric field, for example, determine the conductivity and other such properties. This is also true of a semi-Dirac metal. In particular, the effective mass becomes zero for conduction along a special direction.

“With the advent of man-made 2D materials, such properties have become quite tailorable in what comprises the active field of quantum materials,” says Bhaskaran Muralidharan, from the Electrical Engineering department and one of the authors. “One such example is that the [energy-momentum] dispersion relation can be linear, leading to large velocities and vanishingly small effective masses. The velocities can be over a100 times more than normal metals, thus increasing the mobility and currents that can be carried across devices made of these so-called Dirac materials,” he explains. In the semi-Dirac metals, these properties are direction dependent.

In this paper, the authors have shown theoretically that the direction-dependence of the microscopical properties gives the material special optical properties.

Alongside, the duo also understood that the material should possess interesting thermoelectric properties. “Thermoelectricity is a clean energy technology that uses waste heat to produce electricity typically in low power applications,” says Prof. Muralidharan. This technology is used in efficient cars, where it is used to keep lights on and to warm seats. Spacecrafts like Voyager which are too far from the sun to use solar energy can make use of thermoelectricity. “The holy grail of thermoelectrics is to increase the heat-to electricity conversion efficiency, for which there has been recent and tremendous interest due to the advent of nanomaterials and quantum materials," says Prof. Muralidharan.

In a second paper published as *Rapid Communications* of *Physical Review B,* the researchers show theoretically that semi-Dirac materials can display such thermoelectric properties. This new work paves the way for experimental studies on realising this. The article also describes how to engineer atomic positions and defects to achieve exactly this effect.

The 2019 Nobel Prize for Chemistry was awarded to John B. Goodenough, M. Stanley Whittingham and Akira Yoshino for working towards the development of practical lithium-ion batteries.

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