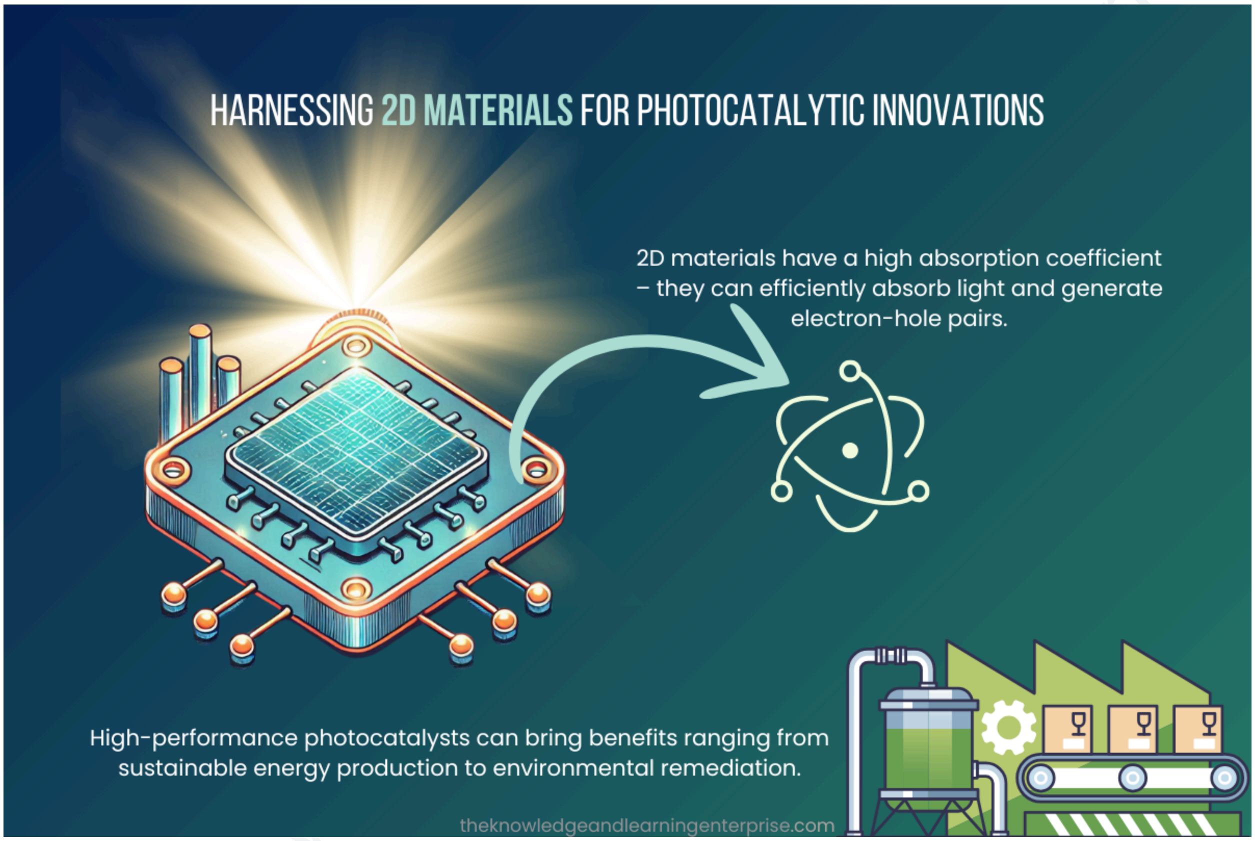
A New Roadmap for High-Performance Photocatalysts Can Help Sustainable Energy Production



A new study offers a roadmap for designing high-performance photocatalysts that can bring benefits ranging from sustainable energy production to environmental remediation.

2D materials have a high absorption coefficient, implying that they can efficiently absorb light and generate electron-hole pairs. This makes them promising candidates for photocatalytic applications. They also have tunable bandgap, reduced path length that charge carriers need to travel, large surface area, and can be easily integrated into various device architectures allowing flexibility and scalability. However, they possess strongly bound excitons (bound state of an electron and an electron hole) and are thus ineffective in driving catalytic reactions that require free charge carriers.

Scientists from the Institute of Nano Science and Technology (INST), Mohali, an autonomous institute of Department of Science and Technology, theoretically studying the ground- and excited-state dynamics of bound electrons-hole pairs (excitons) in a heterostructure of a 2D material called metal-telluric-halide demonstrated that engineering of 2D materials that have high electrical resistivity (dielectric materials) is an efficient strategy to regulate their exciton binding energy (EBE) and could make them efficient catalysts.

In a paper published in the Journal of Physical Chemistry C, they elucidated how the application of a magnetic field accelerates charge separation of such materials by exerting opposing forces on photogenerated electrons and holes. They also enhanced EBE through an exciton diamagnetic shift, which could potentially hinder charge separation.

The highly delocalized exciton cloud extending over a few hundred unit cells reduces the EBE to kBT (25 meV—mili electron volts), promoting spontaneous exciton dissociation into free carriers.

The Scope

Prof. Abir De Sarkar and his PhD Scholars Mr. Amal Kishore and Ms Harshita Seksaria used the PARAM-Smriti supercomputing facility. This facility at NABI is supported by CDAC, Pune under the National Supercomputing Mission, Government of India. They showed that the GaTeCl/InTeBr vdW heterostructure efficiently splits water into hydrogen, providing a clean energy source. The same method can also enable the production of solar fuels like methanol. Additionally, its photocatalytic properties help degrade pollutants, contributing to cleaner air and water.

Reference: New roadmap for high performance photocatalysts can help sustainable energy production