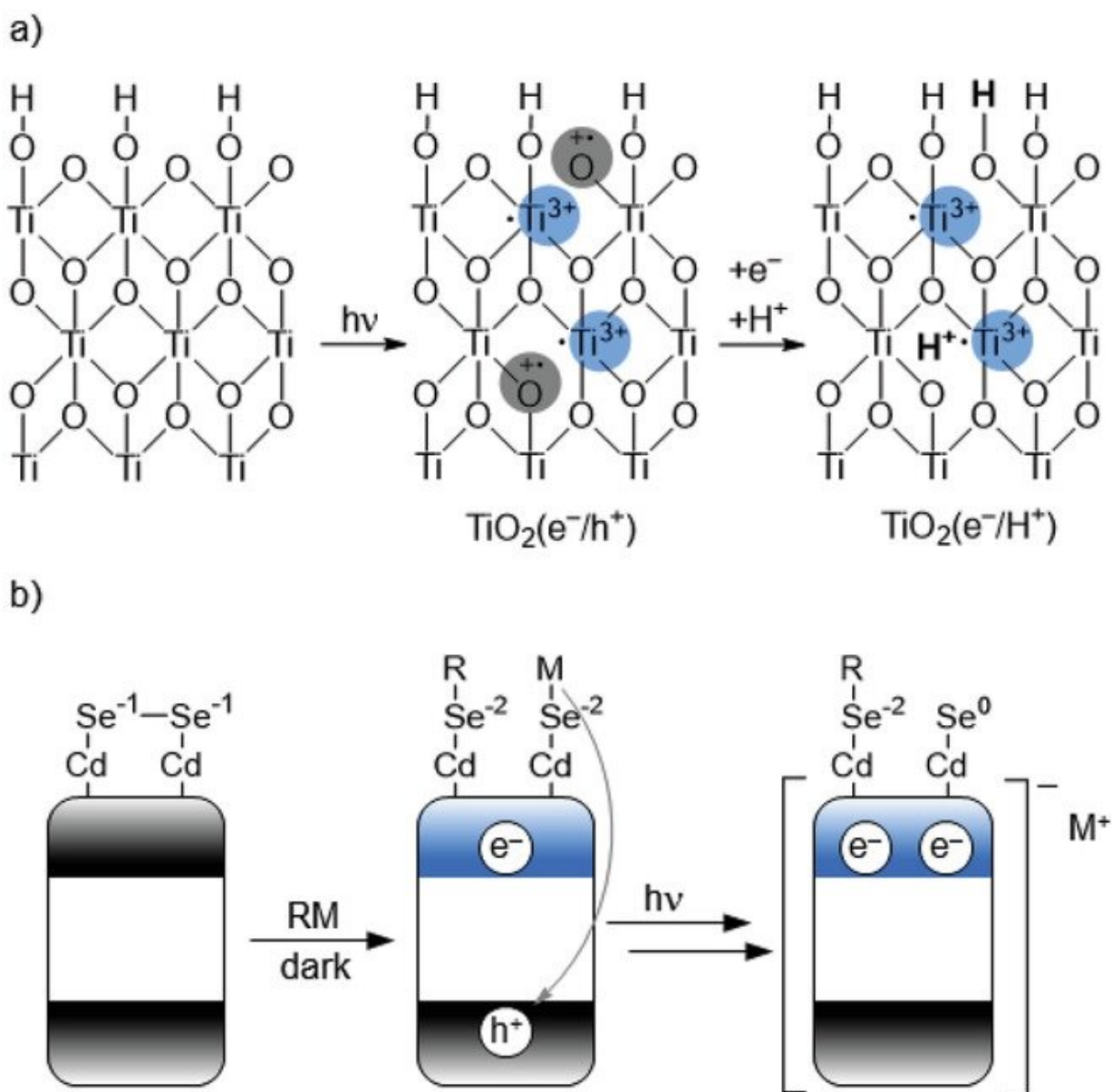


First online database of photocharged materials developed for battery research

October 27 2022, by Juliane Jury



Schematic representation of structural changes in semiconductors exerted by accumulation of electrons and charge-compensating ions. a) A fragment of TiO_2 with surface and bulk Ti^{3+} -sites local structures. b) Changes that occur on the surface of CdSe upon dark prereduction and photocharging. Credit: *Advanced Energy Materials* (2022). DOI: 10.1002/aenm.202200352

Materials chemistry is a rapidly evolving area of research, with thousands of various semiconductors, and more materials being added all the time. What material among this variety would be the best for application in solar batteries, for example? How should such a material look like if it has not yet been synthesized?

To this end, Dr. Aleksandr Savateev has analyzed research data dealing with the charging of [materials](#) by light and compiled their results:

"Scientists generate enormous amount of data. Within a single research article, the data are analyzed, trends are derived and explained. However, comprehensive analysis of data spanning decades of research, even from one field, is very rare. The lack of such analysis ultimately delays the implementation of technological developments—and this is where the database comes in," explains Dr. Savateev.

Forty years ago, a physical phenomenon was observed and studied that could make it possible to combine a light harvester and a battery in one device. Solar farms generate [renewable electricity](#), but [solar panels](#) cannot store it yet. Various [semiconductor](#) materials, including those composed of abundant elements, such as carbon and nitrogen, are photocharged when irradiated with visible light.

Similar to an electric battery, a semiconductor remains charged in the dark for hours and even days, and the energy stored in a photocharged semiconductor may be used on demand for various purposes: "The

database could help find the right semiconductors much quicker," Savateev says.

Photo chargeable semiconductors may not only be used to convert solar light to charge smartphones, research laboratories around the world are using these materials instead of rare elements and expensive reagents to obtain value-added [organic compounds](#).

Organic chemists and materials scientists can use the online database on photocharged materials for their research to select the most suitable semiconductor material. Various filters can be applied to highlight the desired data points according to a specific criterion.

Already, certain trends between the structure of semiconductor materials and their ability for photocharging may be derived from the properties compiled in the database. These dependencies are available in the open access article published in *Advanced Energy Materials*.

About the database

The review summarizes and quantifies [experimental data](#) collected over 40 years of research. Maximum specific concentration of electrons stored in 1 g of a semiconductor, maximum average number of electrons stored per semiconductor particle, initial rate of photocharging, and the initial rate of discharging are calculated for six classes of semiconductor materials: Ti, Zn, Cd, In, W-based, and graphitic carbon nitrides.

Dependence of these parameters on the specific surface area of the material, particle volume, and other properties is analyzed and trends are derived.

A public database of photocharged materials has been created to facilitate design of high-performing materials with photocharging

function, their application as rechargeable reductants in [organic synthesis](#) and the development of devices.

More information: Oleksandr Savateev, Photocharging of Semiconductor Materials: Database, Quantitative Data Analysis, and Application in Organic Synthesis, *Advanced Energy Materials* (2022). DOI: [10.1002/aenm.202200352](https://doi.org/10.1002/aenm.202200352)

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