## A new hub for fresh ideas in materials science

A fast-growing institute associated with China's prestigious Tsinghua University, the Institute of Materials Research has pursued research into FAST AND TARGETED NEW MATERIALS DEVELOPMENT.

## The Institute of Materials

Research (IMR) at Tsinghua Shenzhen International Graduate School (Tsinghua SIGS) is brand new. Established in November 2020, it has a long-term goal of becoming a world leader in fundamental and applied research in the field of materials science and engineering, as well as a place to train and educate the next generation of talent, according to its dean, Hui-Ming Cheng.

Although new, its association with Tsinghua has allowed IMR to attract some notable talent for its founding faculty. "We currently have 20 tenured and tenure-track faculty members as well as around 400 PhD and masters students, which will increase respectively to 50 and 1,000 by 2025," explains Cheng. This influx of top talent will contribute to cross-disciplinary research in IMR's research priorities: material design and computation; materials and devices related to biomedicine, energy, and information science; as well as low-dimensional materials and devices.

"An example of the latter includes our joint study published in *Nature Communications* in 2020, for which my team collaborated with the teams of Andre Geim, at the University of



Na-ion transport mechanism of composite solid-state electrolyte and working mechanism in Na\_3V\_2(PO\_4)\_3 / Na batteries during long cycles

Manchester, and Bilu Liu, at the IMR of Tsinghua SIGS. We demonstrated tunable transmissive magnetocolouration, and discovered a giant magneto-optic effect in two-dimensional crystals," says Cheng. "This research provides a strategy for designing material to tune transmitted colours and can be further applied in the fields where interference colours are of concern."

One of the highest goals in photonics is tuning transmitted interference colours in a noninvasive and contactless way. Interference generated colours are vivid, metallic, with a wide colour range and resistant to photobleaching, compared with interference colours generated by chemical pigments or dyes.

Another 2019 Nature Communications paper by Feiyu Kang's team, the associate dean of SIGS and executive associate dean of IMR, advances sodium batteries, with high working voltage and high energy-density, as an attractive alternative to expensive lithium batteries. Kang's team demonstrated the suppression of sodium dendrite formation, which would otherwise cause safety risks. They constructed hybrid solid/liquid electrolyte of alumina wires with a polymer gel coating, which promoted uniform sodium deposition and formation of a stable and flat solid electrolyte interface on the sodium metal anode. In addition to making sodium batteries more feasible, the work may also have applications for lithium, potassium, or other metal batteries.

## ADVANCING MATERIAL DESIGN AND COMPUTATION

Traditional materials research often uses a process of repeated trial and error without an atomic-level understanding

of structure-property correlations. High-throughput materials simulation and atomic-scale characterization of functional materials, another specialism at IMR, targets the shortcomings of this method. By editing the fundamental elements that control the materials' properties, through electronic structure calculation, mesoscale simulations, transport and dynamic behaviour simulations, and advanced aberration-corrected scanning transmission electron microscopy, materials development can be accelerated.

An example is imaging subsurface hydrogen interstices with an advanced electron microscope. The atomic structure of subsurface interstitial hydrogen remains undetermined, but the absorbed interstitial hydrogen atoms can significantly control the mechanical and chemical properties of metals. An IMR study published in Angewandte Chemie in 2020 reported the first direct imaging of subsurface interstitial hydrogen atoms in palladium hydrides, which have broad application in hydrogen storage and electrocatalysis for energy conversion reactions such as carbon dioxide reduction. By using differential phase contrast with a scanning electron microscope and density functional theory calculations, the researchers predicted the amount and the occupation type of the subsurface hydrogen atoms and were able to finetune the chemical reactivity of palladium surface.



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