TERAHERTZ SPECTROSCOPY

Ionic migration

Nat. Commun. **10**, 2662 (2019)

Ion transport through solids is a fundamental process for the function of many devices, such as fuel cells and batteries. While the past several decades have seen tremendous efforts in discovering new ion-conducting materials, an equally — if not more — important focus is on the fundamental understanding of their conduction mechanism. Now, Morimoto et al. apply terahertz (THz) spectroscopy to track the optical conductivity of an electrolyte at picosecond to nanosecond timescales, revealing otherwise inaccessible information about microscopic ion migration.

The researchers use yttria-stabilized zirconia, a model ionic conductor in which the oxygen vacancies oscillate thermally at a frequency of several THz before hopping to neighbouring sites. On application of THz time-domain spectroscopy, the measured THz conductivity increases monotonically across the frequency range and is confirmed to originate from the strong oscillation of the vacancies. Temperature dependence analysis allows the extraction of the activation energy, which reflects the intrinsic potential barrier the mobile species has to overcome. *YZ*

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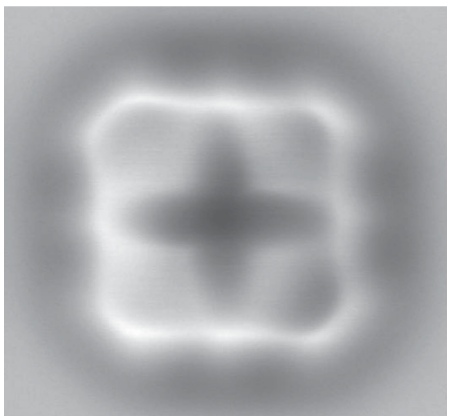
ATOMIC FORCE MICROSCOPY

Changes upon charging

Science **365**, 142–145 (2019)



Credit: AAAS

Charge can induce changes of molecular behaviour in photosynthesis, organic photovoltaic devices and molecular electronics. Existing characterization techniques such as X-ray diffraction and vibrational and optical microscopy can only provide us with the average information of a large number of molecules. Now, Fatayer et al. use Atomic Force Microscopy (AFM) to monitor changes on the single-molecule level upon charging and discharging.

They adsorb four different molecules on insulating NaCl multilayers, which allows them to study the molecules in different charge states. Controlled transfer of electrons from/to the CO functionalized AFM tip charges/discharges the molecule. High-resolution AFM images unveil changes in molecular conformation, bond order and aromaticity in multiple charge states. They find that the addition of electrons distorts azobenzene from planar to non-planar. The change of bond lengths in the dianion pentacene suggests the formation of radical anions in its second and fourth rings. The AFM and DFT results reveal changes in the geometry of dicyano moieties in tetracyanoquinodimethane upon charge-state changes. Furthermore, they observe changes of the aromaticity and conjugation pathway of porphine with altering bond order at different oxidation states. *WS*

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MACHINE LEARNING

The machine unveils

Nature **570**, 484–490 (2019)

We as humans are fairly good at recognizing faces, even in fuzzy images, but would likely fail to detect correlation and order in images of complex, noisy data. While Fourier analysis often helps, it also fails if the disorder is too strong. Zhang et al. now demonstrate how machine learning using artificial neural networks (ANNs) can identify hidden order in experimental data of electronic quantum matter, such as high-temperature superconductors or quantum spin liquids, which cannot be unveiled with traditional methods.

The researchers analyse sets of differential conductance maps obtained by scanning tunnelling microscopy experiments on carrier-doped copper oxide Mott insulator samples. The strong atomic-scale disorder in such samples commonly prohibits recognition of periodic electron density variations and the determination of the quantum state. Zhang et al. first train the ANNs with synthetic images representing different order, commensurate or not with the atomic lattice of the crystal, but including disorder and defects. Then, the researchers run them on sets of experimental images of several samples with different doping levels. The machine learning algorithm recognizes a lattice-commensurate, symmetry-breaking order, which provides experimental evidence to distinguish between competing theoretical models to describe this Mott insulator. *BH*

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2D PEROVSKITES

Current on the edge

Sci. Adv. **5**, eaau3241 (2019)

Owing to their enhanced photostability, two-dimensional (2D) halide perovskites are posed to impact the field of perovskite optoelectronics. In 2D perovskites that form a typical multiple quantum well (MQW) structure, the presence of strong quantum confinement effects largely affects the charge transport and photophysics of the material system. To provide much needed further insights into these phenomena, Wang et al. investigate the edges of 2D perovskite heterolayers.

The researchers synthesize single crystal MQW perovskite thin films and characterize their top layers by conducting atomic force microscopy. While the bulk terrace region of the samples shows insulating properties, an unexpectedly strong current is detected along the contour of the layer edges. The increase in current at the sharp layer edges can be attributed to the free charge carriers residing at the edge states. Scanning electron microscopy, confocal Raman and photoluminescence measurements confirm that the observed feature cannot be ascribed to chemical compounds at the edges or surface charge accumulation and instead is intrinsic in nature. Furthermore, the current is not sensitive to illumination — it changes polarity depending on the scan direction and is characterized by a metal-like carrier density. *OB*

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