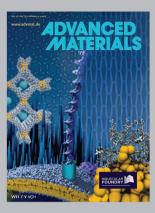
# ADVANCED FUNCTIONAL MATERIALS

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#### Saddle Structures

Using a complex power amplification system, mantis shrimps ulitize a saddle-shaped biospring to store and quickly release elastic energy, enabling them to deliver deliver ultra-fast strikes on their prey. On page 6437, A. Miserez and coworkers demonstrate that the saddle is a bi-layer material with distinct degrees of mineralization. One layer is used to maximize elastic energy storage during loading, while the other layer provides flexibility and prevents fracture during repeated loading/unloading cycles.



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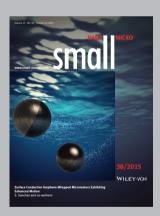
#### **Photothermal Ablation**

As shown on page 6527, an effective, near-infrared (NIR)-responsive rattle-type  $\text{Fe}_3\text{O}_4$ @CuS nanoparticle containing delocalized  $\text{Fe}_3\text{O}_4$  nanoparticles inside a hollow porous CuS structures is developed by C.-S. Yeh and co-workers for magnetic resonance imaging diagnosis and magnetically guided photothermal tumor ablation applications in the first and second NIR biological windows. The nanoparticle features a magnetic target, magnetic resonance imaging diagnosis, and photothermal therapy functions through the manipulation of a magnet and NIR laser.



#### **Porous Coordination Polymers**

On page 6448, S.-Q. Zang and co-workers report a water-triggered diplex structural transformation involving both single-crystal to single-crystal and dissolution–recrystallization processes from a standard 2D Kagomé lattice to a 3D NbO network via a distorted Kagomé lattice structural intermediate. Excitingly, the final product preferentially absorbs water over alcohol, enabling technological applications in high-efficiency separation of water and alcohol.

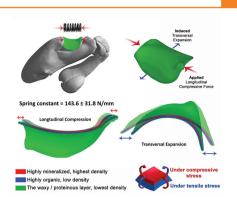


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Mantis shrimps deliver ultrafast strikes using a complex power amplification system, within which the "saddle biospring" is used to store and quickly release the elastic energy. It is demonstrated that the saddle is a bilaver material with distinct degrees of mineralization. One layer is used to maximize elastic energy storage during loading, while the other layer provides flexibility and prevents fracture.

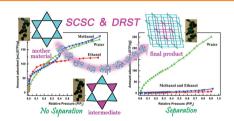


#### Saddle Structures

M. Tadayon, S. Amini, A. Masic, A. Miserez\*.....6437-6447

The Mantis Shrimp Saddle: A Biological Spring Combining Stiffness and Flexibility

A water-triggered diplex structural transformation is successfully implemented porous coordination polymers (PCPs), the mechanism of which is definitely clarified by the isolated and characterized intermediate. More excitingly, thanks to its high-efficiency separation of water from alcohol the final product has a myriad of potential applications in separation technology.

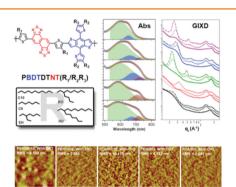


#### **Porous Coordination Polymers**

L.-H. Cao, Y.-S. Wei, H. Xu, S.-Q. Zang,\* T. C. W. Mak.....6448-6457

Unveiling the Mechanism of Water-Triggered Diplex Transformation and Correlating the Changes in Structures and Separation Properties

Systematic side chain engineering based on naphtho [1,2-c:5,6-c]bis[1,2,5] thiadiazole-benzodithiophene copolymer is carried out; a detailed structural analysis of these polymers in the active layer of organic solar cells is performed to elucidate the influence of side chain on their crystalline, morphological, and photovoltaic properties.

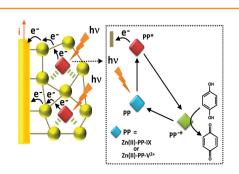


#### Solar Cells

P. Liu, S. Dong, F. Liu, \* X. Hu, L. Liu, Y. Jin, S. Liu, X. Gong, T. P. Russell,\* F. Huang,\* Y. Cao ......6458-6469

**Optimizing Light-Harvesting Polymers** via Side Chain Engineering

The structural features of Zn(II)-protoporphyrin IX or bipyridinium-modified Zn(II)-protoporphyrin IX are imprinted in electropolymerized bis anilinecrosslinked Au nanoparticle matrices associated with electrodes. The concentration of the photosensitizers at the electrodes by means of the imprinted sites leads to effective charge separation resulting in intensified photocurrents.



### Electropolymerization

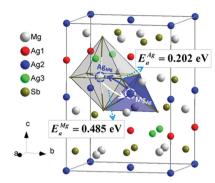
T. S. Metzger, R. Tel-Vered, H. B. Albada, I. Willner\*.....6470-6477

Zn(II)-Protoporphyrin IX-Based Photosensitizer-Imprinted Au-Nanoparticle-Modified Electrodes for Photoelectrochemical Applications

#### Thermoelectric Materials

D. Li, H. Zhao, \* S. Li, B. Wei, J. Shuai, C. Shi, X. Xi, P. Sun, S. Meng, L. Gu, Z. Ren,\* X. Chen\* ...... 6478-6488

Atomic Disorders Induced by Silver and Magnesium Ion Migrations Favor High Thermoelectric Performance in α-MgAgSb-Based Materials

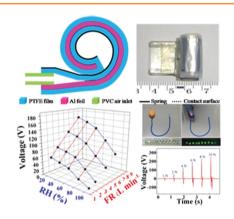


The underlying mechanism responsible for the high thermoelectric performance in α-MgAgSb-based materials is disclosed. Based on density function theory calculations and experimental characterizations, concurrent silver and magnesium ion migrations are revealed in  $\alpha$ -MgAgSb. This is believed to be the origin of the low thermal conductivity in  $\alpha$ -MgAgSb-based materials and plays an important role in the good figure of merit of these materials.

#### **Multifunctional Sensors**

M. Ma, Q. Liao, G. Zhang, Z. Zhang, Q. Liang, Y. Zhang\*.....6489-6494

**Self-Recovering Triboelectric** Nanogenerator as Active Multifunctional Sensors



A novel self-recovering triboelectric nanogenerator (STENG) is developed and serves as a multifunctional sensor. The STENG has self-recovering and rollable characteristics due to the spring assembled into the nanogenerator. The output performance is extremely high. It can be utilized as self-powered multifunctional sensors to detect humidity, airflow rate, and motion.

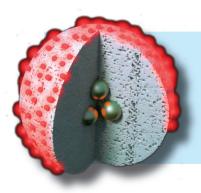
#### **Molecular Screening**

E. O. Pyzer-Knapp, K. Li, A. Aspuru-Guzik\*......6495-6502

Learning from the Harvard Clean Energy Project: The Use of Neural Networks to **Accelerate Materials Discovery** 

The utility of including neural networks as a highly accurate screening function is demonstrated for molecules from the Harvard Clean Energy Project. The neural network described can predict power conversion efficiencies of molecules with an error of 0.12%. By using this network as a screen for generated molecules, the scope of highthroughput virtual screening is expanded by several orders of magnitude.





#### How to contact us:

#### **Editorial Office:**

Phone: (+49) 6201-606-286/531 Fax: (+49) 6201-606-500 Email: afm@wiley-vch.de

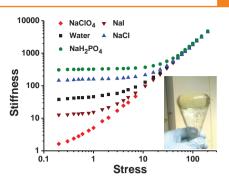
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Salts are known to change the interactions between water and polymers and consequently change transition temperatures, an effect known as the Hofmeister effect. It is shown that beyond phase transition temperatures, ions can be used to tailor the linear and nonlinear mechanical behavior of hydrogels. A hundredfold stiffness increase is realized with gels of identical morphology.

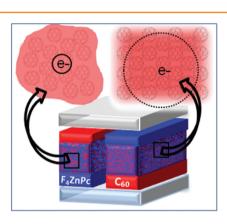


#### Hydrogels

M. Jaspers, A. E. Rowan,\* P. H. J. Kouwer\*.....6503-6510

Tuning Hydrogel Mechanics Using the Hofmeister Effect

Substrate-induced local fullerene ordering is found in small molecule: C60 bulk heterojunctions (BHJs) deposited on pristine C<sub>60</sub> at elevated temperatures. This does not occur for BHJs deposited under identical conditions on pristine donor molecule layers, despite similar degrees of phase separation in both cases. These findings point to a hitherto unidentified advantage of inverted over noninverted solar cells that manifests itself in a higher charge separation efficiency.

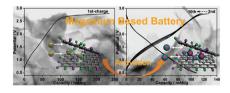


#### **Organic Photovoltaics**

D. Nanova, M. Scherer, F. Schell, J. Zimmermann, T. Glaser, A. K. Kast, C. Krekeler, A. Pucci, W. Kowalsky, R. R. Schröder.\* R. Lovrinčić\*... 6511-6518

Why Inverted Small Molecule Solar Cells Outperform Their Noninverted Counterparts

A fast surface redox process is proposed to replace sluggish lattice migration for improving the performance of Mg based batteries. The proof-of-concept Mg/ fluorinated graphene nanosheet system is activated by a prior anionic process followed by reversible cationic storage with a capacity higher than 100 mAh g-1 in a pseudocapacitance behavior from 2.75 to 0.5 V.

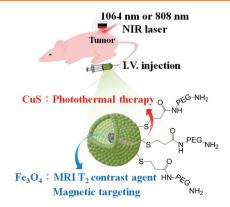


#### **Magnesium Batteries**

J. Xie, C. Li,\* Z. Cui, X. Guo ... 6519-6526

Transition-Metal-Free Magnesium-Based **Batteries Activated by Anionic Insertion** into Fluorinated Graphene Nanosheets

effective, near-infrared (NIR)responsive rattle-type Fe<sub>3</sub>O<sub>4</sub>@CuS nanoparticle is developed to conduct magnetically guided photothermal tumor ablation and magnetic resonance imaging diagnosis through magnetic targeting. Based on the broad NIR absorption from 700 to 1300 nm, photothermal tumor ablation is evaluated by radiation at 808 and 1064 nm of the first and second NIR windows, respectively.



#### **Photothermal Ablation**

Z.-C. Wu, W.-P. Li, C.-H. Luo, C.-H. Su, C.-S. Yeh\* ......6527-6537

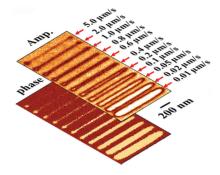
Rattle-Type Fe<sub>3</sub>O<sub>4</sub>@CuS Developed to Conduct Magnetically Guided Photoinduced Hyperthermia at First and Second NIR Biological Windows

#### Ferroelectric Films

P. Sharma, \* S. Ryu, Z. Viskadourakis, T. R. Paudel, H. Lee, C. Panagopoulos. E. Y. Tsymbal, C.-B. Eom,

A. Gruverman\* 6538–6544

Electromechanics of Ferroelectric-Like Behavior of LaAlO3 Thin Films

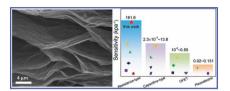


Electrically and mechanically induced ferroelectric-like polar states are investigatedIn the ultrathin LaAlO3 films, using a combination of scanning probe microscope techniques. The ferroelectric-like behavior is associated with the reorganization of oxygen vacancies between the two stable states, which can be controlled at the submillisecond timescale using either the electrical or the mechanical stimulus

#### **Graphene Sensors**

L. Sheng, Y. Liang, L. Jiang, Q. Wang, T. Wei, L. Qu,\* Z. Fan\*........ 6545-6551

**Bubble-Decorated Honeycomb-Like** Graphene Film as Ultrahigh Sensitivity **Pressure Sensors** 



A flexible, bubble-decorated, honeycomblike graphene film (BHGF) is fabricated by a low-temperature heat treatment of graphene oxide film. The as-prepared BHGF exhibits an ultrahigh sensitivity of 161.6 kPa<sup>-1</sup> at a strain less than 4%, due to the switching effect depended on "point-to-point" and "point-to-face" contact modes.

