# ADVANCED FUNCTIONAL MATERIALS

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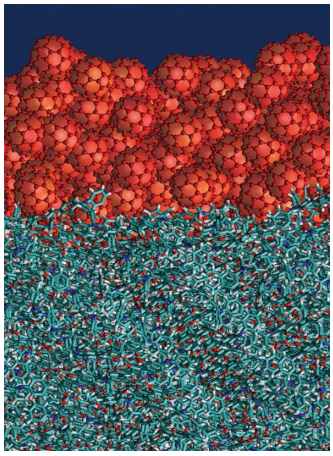
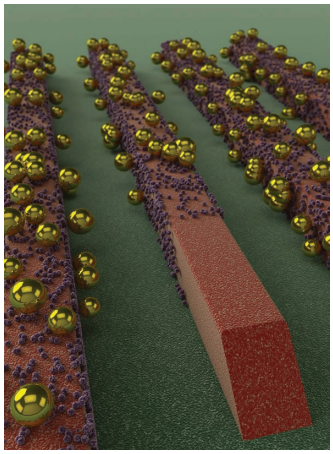


**Interfaces**

Theoretical models of the squaraine-$C_{60}$ donor–acceptor interface reported on page 3790 by C. Risko, J.-L. Brédas, and co-workers probe how molecules pack, mix, and move and the subsequent impact on interfacial electronic properties of organic solar cells. The 3D molecular shape, disordered packing, and thermal motion at room temperature render electronic couplings small, regardless of the orientation of the underlying squaraine layers. Such insight is vital to develop a more robust understanding of the photoconversion process and offers principles for materials design.

**Crystallization**

Top-down e-beam lithography is combined with bottom-up bioinspired crystal growth by R. de la Rica, M. M. Stevens, and co-workers to grow nanoparticle clusters of controlled dimensions at desired locations on a chip. On page 3692, the key enabling factor to recreate biomineralization conditions is the patterning of enzyme nanoreactors as lines separated by nanometric distances such that the gradient of crystallization precursors generated by the enzymes is affected by the nanoscale organization of biocatalysts. Image Credit: Miguel Spuch-Calvar.



**Thermochromic Sensors**

A new type of bis-polydiacetylene (PDA), in which two PDAs are linked via an intervening p-phenylene group, displays excellent thermochromic reversibility. Clear blue-to-red and red-to-blue colorimetric transitions are observed by R. Chang, J. Yoon, and co-workers between 20 and 120 °C. The first theoretical simulation of the new PDA is reported on page 3699, the results of which successfully explain the thermochromic reversibility phenomenon.

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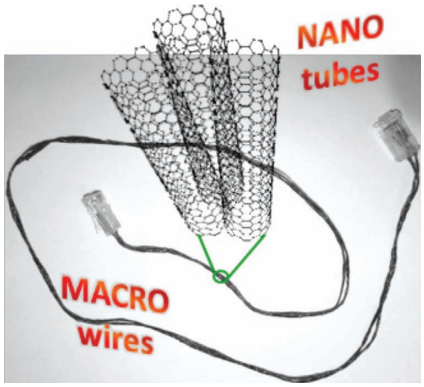
## FEATURE ARTICLE

### Electrical Wires

A. Lekawa-Raus, J. Patmore, L. Kurzepa, J. Bulmer, K. Koziol* ..... 3661–3682

**Electrical Properties of Carbon Nanotube Based Fibers and Their Future Use in Electrical Wiring**



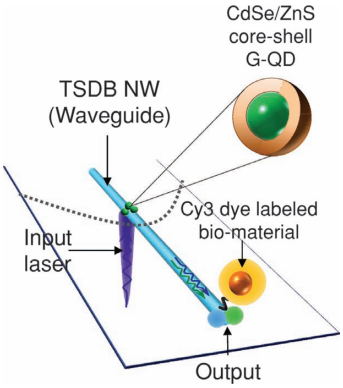

**Carbon nanotubes**, with their unique properties, could make electrical conductors of unprecedented performance, which could revolutionize energy transport globally. Is it feasible to produce macroscopic conductors from nanoscale structures? This Feature Article presents both the most recent results of a highly promising research program in this area and the key challenges that need to be overcome.

## FULL PAPERS

### Optical Waveguiding

E. H. Cho, B.-G. Kim, S. Jun, J. Lee, D. H. Park, K.-S. Lee, J. Kim,* J. Kim,* J. Joo* ..... 3684–3691

**Remote Biosensing with Polychromatic Optical Waveguide Using Blue Light-Emitting Organic Nanowires Hybridized with Quantum Dots**



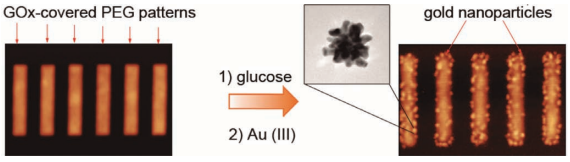

**Nanoscale polychromatic optical waveguides** are demonstrated using a novel hybrid composite of highly crystalline blue light-emitting organic nanowires (NWs) combined with blue, green, and red CdSe/ZnS quantum dots (QDs). The transportation of QD-emission through the highly packed $\pi$-conjugated organic NW enhanced the remote biosensing signal.

### Crystallization

R. de la Rica,* E. Bat, K. L. Herpoldt, H.-n. Xie, S. Bertazzo, H. D. Maynard, M. M. Stevens* ..... 3692–3698

**Nanoparticle Growth via Concentration Gradients Generated by Enzyme Nanopatterns**

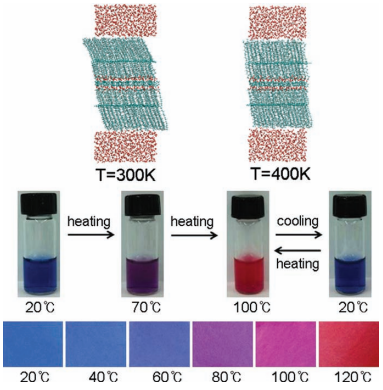
**Concentrations gradients generated by enzyme patterns** guide the growth of gold nanostructures with programmable size, shape, and state of aggregation. When the patterns are separated by nanometric distances, clusters of highly crystallographically aligned gold nanoscrystals are obtained, which suggests that the nanoparticles grow via biomimetic non-classical crystal growth conditions.




### Thermochromic Sensors

S. Lee, J. Lee, M. Lee, Y. K. Cho, J. Baek, J. Kim, S. Park, M. H. Kim, R. Chang,* J. Yoon* ..... 3699–3705

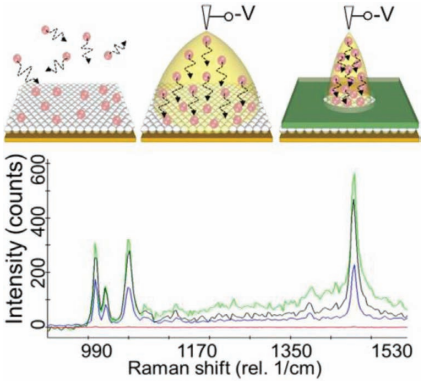
**Construction and Molecular Understanding of an Unprecedented, Reversibly Thermochromic Bis-Polydiacetylene**




**The Bis-PDA-Ph (two PDAs are linked via an intervening *p*-phenylene group)** displays exceptional thermochromic reversibility with a blue to red colorimetric transition at elevated temperatures. To elucidate the molecular origin of the thermochromic response, a theoretical simulation of the new PDA which explains the reversibility phenomenon, is conducted. Furthermore, Bis-PDA-Ph-embedded fibers display excellent reversibility between 20–120 °C.

## FULL PAPERS

**In the field of sensors that target the detection of airborne analytes**, the corona/lens-based-collection provide a new path to achieve high sensitivity which impacts the researches ranging from environmental monitoring systems to the detection of chemical/biological warfare agents. Specifically, it provides a route to transport, concentrate, and collect the airborn species to precise sensing points to improve the collection efficiency.

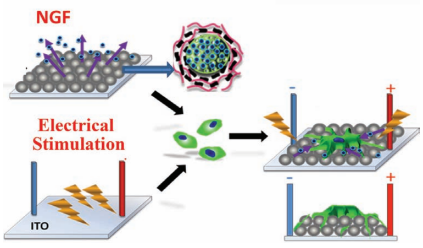



### Gas Sensors

J. Fang, S.-C. Park, L. Schlag, T. Stauden, J. Pezoldt, H. O. Jacobs*.....3706–3714

**Localized Collection of Airborne Analytes: A Transport Driven Approach to Improve the Response Time of Existing Gas Sensor Designs**

**The stimulus-responsive, well-ordered $rGO_{SH}/PMA_{SH}$ microcapsules** are arrayed into a 3-D ECM-mimic flexible substrate to accelerate the proliferation and differentiation of PC12 cells by controlling NGF release and manipulating $rGO_{SH}/PMA_{SH}$ microcapsule interfaces. A combination of surface topography, chemical cues, and electrical stimulation not only has positive effects on cell viability but also strongly enhances the neurite outgrowth of PC12 cells.

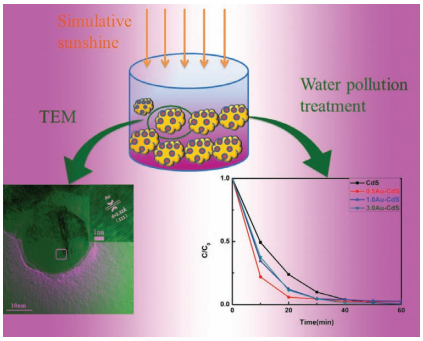



### Neural Cells

H.-W. Liu, W.-C. Huang, C.-S. Chiang, S.-H. Hu, C.-H. Liao, Y.-Y. Chen,* S.-Y. Chen* .....3715–3724

**Arrayed $rGO_{SH}/PMA_{SH}$ Microcapsule Platform Integrating Surface Topography, Chemical Cues, and Electrical Stimulation for Three-Dimensional Neuron-Like Cell Growth and Neurite Sprouting**

**The CdS SNPs-Au NPs hybrids** are firstly fabricated through gold-sulfur bonding interaction, which meets the needs for reliable interfacial contact between the semiconductor and Au NPs. This facile strategy can be extended to the synthesis of other binary semiconductor hybrids. The as-fabricated CdS SNPs-Au NPs hybrids are very promising for application in degradation of organic pollutants.

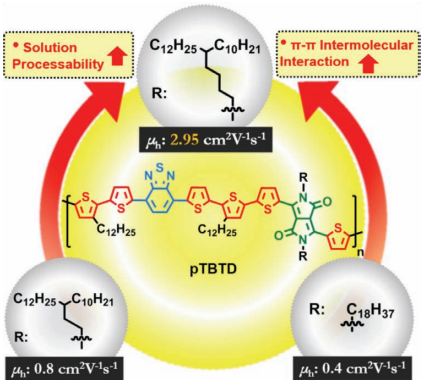



### Semiconductor Photocatalysts

S. C. Han, L. F. Hu, N. Gao, A. A. Al-Ghamdi, X. S. Fang*...3725–3733

**Efficient Self-Assembly Synthesis of Uniform CdS Spherical Nanoparticles-Au Nanoparticles Hybrids with Enhanced Photoactivity**

**5-Decylheptadecyl (5-DH), 2-tetradecyl (2-DT), and *n*-octadecyl (OD) side chains** are substituted into pTBTD polymer backbone. The branching position is remote or close to pTBTD in 5-DH and 2-DT. 5-DH merges advantages of branched units (2-DT) for improving solubility with those of linear chains (OD) in providing effective $\pi$–$\pi$ intermolecular interactions. 5-DH substituted pTBTD exhibits a field-effect hole mobility reaching 2.95 $cm^2\ V^{-1}\ s^{-1}$.




### Polymer Semiconductors

B. Fu, J. Baltazar, A. R. Sankar, P.-H. Chu, S. Zhang, D. M. Collard, E. Reichmanis* .....3734–3744

**Enhancing Field-Effect Mobility of Conjugated Polymers Through Rational Design of Branched Side Chains**

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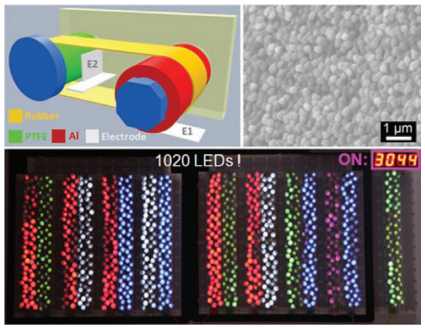
## Energy Harvesting

Y. Yang, H. Zhang,
Z. L. Wang* ..... 3745–3750

**Direct-Current Triboelectric Generator**

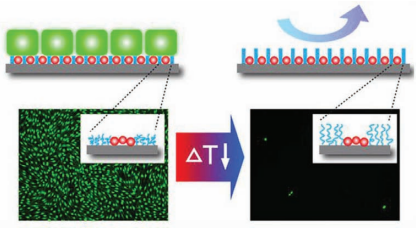



**The first direct-current triboelectric generator (DC-TEG) for harvesting mechanical energy** from rotational motion is reported. The DC-TEG consists of two rotating wheels and one belt for connecting them, which are made of different triboelectric materials. The DC-TEG can be utilized to light up 1020 commercial LEDs and the produced energy can also be stored in a capacitor for other uses.

## Polymer Brushes

Q. Yu, L. M. Johnson,
G. P. López* ..... 3751–3759

**Nanopatterned Polymer Brushes for Triggered Detachment of Anchorage-Dependent Cells**

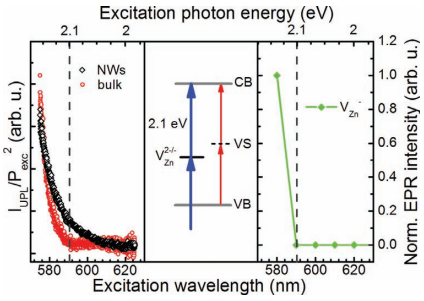



**Thermoresponsive poly(*N*-isopropylacrylamide) (PNIPAAm) brushes** are nanopatterned via interferometric lithography and surface-initiated polymerization to support mammalian cell harvesting. Above the lower critical solution temperature (LCST), collapsed PNIPAAm brushes expose extracellular matrix proteins on the underlying substrate to support cellular attachment. As the temperature decreases below the LCST, swollen, extended PNIPAAm nanopatterned brushes readily release attached cells.

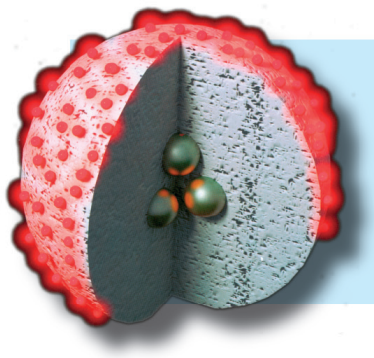
## Semiconductors

J. E. Stehr, S. L. Chen, N. K. Reddy,
C. W. Tu, W. M. Chen,
I. A. Buyanova* ..... 3760–3764

**Turning ZnO into an Efficient Energy Upconversion Material by Defect Engineering**




**ZnO** can be engineered via a common intrinsic defect into an efficient energy upconversion material. This finding paves the way for designing ZnO devices in which the energy upconversion can be exploited for improved and new photonic and photovoltaic applications.



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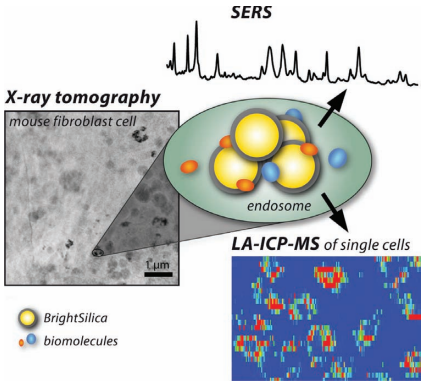
## FULL PAPERS

**BrightSilica nanoparticles have a silica surface and a gold core.** They provide information about their interaction with biological cells via three different approaches: 1) surface-enhanced Raman scattering for characterization of the biomolecular species interacting with the silica sub-/surface; 2) quantification of the uptake of silica-like nanostructures by mass spectrometric micromapping, and; 3) understanding the 3D subcellular interaction using synchrotron X-ray nanotomography.

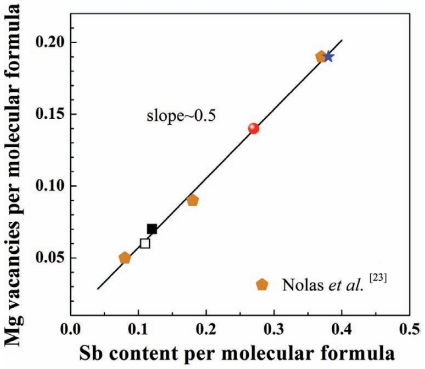



### Silica Nanoparticles

D. Drescher, I. Zeise, H. Traub, P. Guttmann, S. Seifert, T. Büchner, N. Jakubowski, G. Schneider, J. Kneipp*.....3765–3775

**In situ Characterization of $SiO_2$ Nanoparticle Biointeractions Using BrightSilica**

**A new point defect chemistry approach** is proposed for enhancing thermoelectric properties, and demonstrated in typical $Mg_2(Si,Sn)$ based thermoelectric materials via synergistically implementing the point defects of Sb dopants, Mg vacancies, and Mg interstitials. High doping ratio of Sb facilitates the formation of Mg vacancies, which act as both acceptors and phonon scatters, and significantly reduce the lattice thermal conductivity.

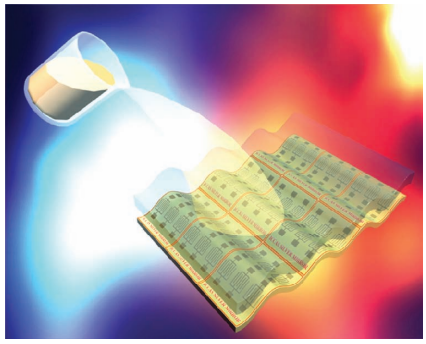



### Thermoelectricity

G. Y. Jiang, J. He, T. J. Zhu,* C. G. Fu, X. H. Liu, L. P. Hu, X. B. Zhao* .....3776–3781

**High Performance $Mg_2(Si,Sn)$ Solid Solutions: a Point Defect Chemistry Approach to Enhancing Thermoelectric Properties**

**Large-area, flexible, high-performance all-solution-processed polymer field-effect transistors** are fabricated with bottom-contact configuration with the help of "regioselectivity deposition" method. The polymer devices exhibit high performance (the highest mobility up to 1.5 $cm^2\ V^{-1}\ s^{-1}$) and excellent environmental stability and flexibility, indicating the cost effectiveness of this method for practical applications in organic electronics.

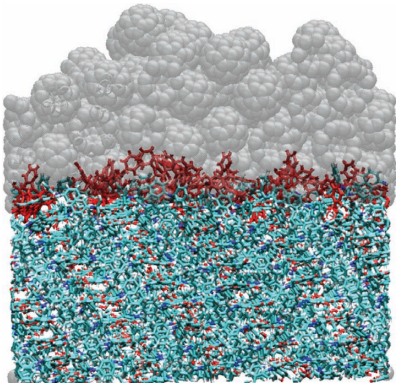


### Organic Electronics

D. Ji, L. Jiang,* Y. Guo, H. Dong,* J. Wang, H. Chen, Q. Meng, X. Fu, G. Tian, D. Wu, G. Yu,* Y. Liu, W. Hu* .....3783–3789

**"Regioselective Deposition" Method to Pattern Silver Electrodes Facilely and Efficiently with High Resolution: Towards All-Solution-Processed, High-Performance, Bottom-Contacted, Flexible, Polymer-Based Electronics**

**A combined molecular dynamics–quantum mechanics approach** reveals the complex landscape of the intermolecular electronic couplings at the squaraine–$C_{60}$ (donor–acceptor) bilayer interface as a function of the interfacial molecular packing and dynamics. Such aspects are of importance when considering the operation of organic solar cells.



### Interfaces

Y.-T. Fu, D. A. da Silva Filho, G. Sini, A. M. Asiri, S. G. Aziz, C. Risko,* J.-L. Brédas* .....3790–3798

**Structure and Disorder in Squaraine–$C_{60}$ Organic Solar Cells: A Theoretical Description of Molecular Packing and Electronic Coupling at the Donor–Acceptor Interface**

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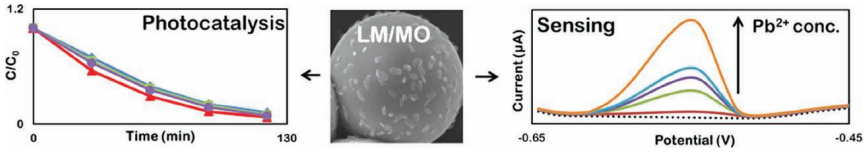
W. Zhang,* J. Z. Ou, S.-Y. Tang, V. Sivan, D. D. Yao, K. Latham, K. Khoshmanesh, A. Mitchell, A. P. O'Mullane, K. Kalantar-zadeh* ..... 3799–3807

**Liquid Metal/Metal Oxide Frameworks**

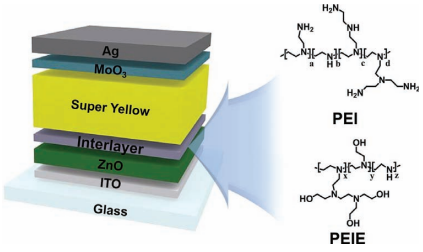
**A new platform described as the liquid metal/metal oxide (LM/MO) framework** is introduced. The constituent spherical structures of these frameworks are made of micro- to nanosized liquid metal spheres and nanosized metal oxides. These LM/MO frameworks demonstrate high sensitivity towards low concentrations of heavy metal ions and enhanced solar light driven photocalalytic activities.




## Polymer Interlayers

Y.-H. Kim, T.-H. Han, H. Cho, S.-Y. Min, C.-L. Lee, T.-W. Lee* ..... 3808–3814

**Polyethylene Imine as an Ideal Interlayer for Highly Efficient Inverted Polymer Light-Emitting Diodes**

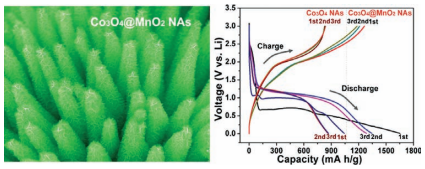



**Efficient and air-stable inverted polymer-light emitting diodes (IPLEDs)** can be realized by using insulating polymer electron-injecting interlayers (ILs), branched polyethyleneimine (PEI), and polyethyleneimine ethoxylated (PEIE), giving highest current efficiencies of 13.5 cd $A^{-1}$ and 12 cd $A^{-1}$, respectively. Polymer ILs can facilitate electron injection into emitting layer as well as block the exciton quenching.

## Supercapacitors

D. Kong, J. Luo, Y. Wang, W. Ren, T. Yu, Y. Luo, Y. Yang, C. Cheng* ... 3815–3826

**Three-Dimensional $Co_3O_4$@$MnO_2$ Hierarchical Nanoneedle Arrays: Morphology Control and Electrochemical Energy Storage**

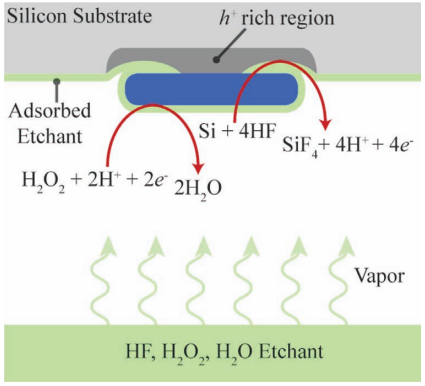



**Highly ordered $Co_3O_4$@$MnO_2$ hierachical core–shell arrays on Ni foam** are fabricated by a facile, stepwise hydrothermal approach and further investigated as anodes for both supercapacitors and Li-ion batteries (LIBs), which present greatly improved performance.

## Chemical Etching

O. J. Hildreth,* D. R. Schmidt ..... 3827–3833

**Vapor Phase Metal-Assisted Chemical Etching of Silicon**




**To overcome non-uniformity and microporous silicon generation** seen in traditional liquid-phase metal-assisted chemical etching, vapor-phase metal-assisted chemical etching (VP-MaCE) is used instead. The etch rate is evaluated as a function of catalyst, time, and substrate temperature.