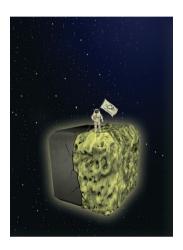
# ADVANCED FUNCTIONAL MATERIALS

## www.afm-journal.de



#### Zeolites

On page 1923 Javier Pérez-Ramírez and coworkers establish methods involving acid and optionally base treatments to prepare hierarchical FAU and LTA-type zeolites. By conquering the latter Al-rich frameworks, the full compositional and topological flexibility desired in the design of hierarchical zeolites by post-synthetic strategies is accomplished. Upon functionalization, the mesoporous X, Y, and A zeolites display superior performance as base catalysts. Carolina Flores is acknowledged for perfecting the cover artwork.



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#### Thin Films

On page 1957 Barbara Scherrer and co-workers report changes in electrical conductivity at low temperatures that occur when grain size, grain shape, and the porosity of nanoporous zirconia-based thin films are varied. The cover image shows a false-colored scanning transmission electron microscopy (STEM) image of a yttria stabilized zirconia (YSZ) thin film with a thickness of about 300 nm contacted with platinum. The bright areas within the YSZ thin film are pores, which conduct protons at temperatures below 400 °C.



#### Carbon Nanotubes

On page 1883 Markus J. Buehler, Horacio D. Espinosa, and co-workers report a study designed to probe the interfacial shear strength between carbon nanotube (CNT) bundles, which is a key element in the bottom-up hierarchical design of CNT fibers with unprecedented mechanical performance. The back cover image blends renderings from atomistic and coarse-grain molecular dynamics simulations with scanning electron microscopy images of shearing between surface-functionalized doublewalled nanotube (DWNT) bundles. The background shows a mat of CNT bundles from which a pair of bundles is selected for testing.



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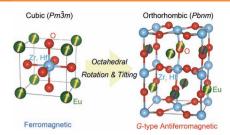
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#### **FULL PAPERS**

#### **Perovskites**

H. Akamatsu,\* Y. Kumagai, F. Oba, K. Fujita, K. Tanaka, I. Tanaka......1864-1872

Strong Spin-Lattice Coupling Through Oxygen Octahedral Rotation in **Divalent Europium Perovskites** 

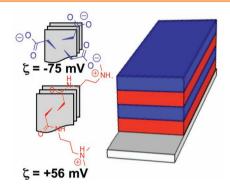


First-principles calculations reveal that in divalent europium perovskites EuMO3 (M = Ti, Zr, and Hf), antiferomagnetic superexchange interactions via *nd* states of the B-site M cations (n = 3, 4, and 5,respectively) are enhanced by rotations of the MO<sub>6</sub> octahedra. The octahedral rotations involved in a structural change from cubic Pm3m to orthorhombic Pbnm structures point the M nd orbitals at the Eu sites, leading to a significant overlap between the M nd and Eu 4f orbitals.

#### Graphene

S. A. Sydlik, T. M. Swager\*.....1873-1882

Functional Graphenic Materials Via a Johnson-Claisen Rearrangement

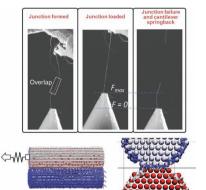


The hydroxyl functionalities in graphene oxide (GO) are subjected to Johnson-Claisen rearrangement conditions, which trades the labile CO bond for a robust CC bond. Further functionalization allows for the synthesis of highly charged, water-soluble graphene. The negatively and positively charged graphenes (zeta potentials of -75 mV and +56 mV), are successfully used to build layer-by-layer (LBL) constructs.

#### **Carbon Nanotubes**

M. Naraghi, G. H. Bratzel, T. Filleter, Z. An, X. Wei, S. T. Nguyen, M. J. Buehler,\* H. D. Espinosa\*.....1883-1892

**Atomistic Investigation of Load** Transfer Between DWNT Bundles "Crosslinked" by PMMA Oligomers



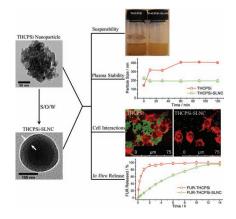
In situ chemical vapor deposition functionalization of CNT bundles by PMMAlike oligomers enhances the shear strength of the bundle junctions by about an order of magnitude compared with "bare" van der Waals (vdW) interactions between pristine CNTs. Through a combination of nanomechanics experimental studies and multiscale simulations, the enhancement of shear strength is attributed to an interlocking mechanism of polymer chains in the bundles, dominated by vdW interactions, and stretching and alignment of chains during shearing.

#### **Drug Delivery**

D. F. Liu, E. Mäkilä, H. B. Zhang, B. Herranz, M. Kaasalainen, P. Kinnari, J. Salonen, J. Hirvonen,

H. A. Santos\*.....1893-1902

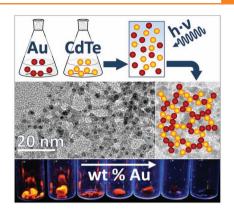
Nanostructured Porous Silicon-Solid Lipid Nanocomposite: Towards **Enhanced Cytocompatibility and** Stability, Reduced Cellular Association, and Prolonged Drug Release



Thermally hydrocarbonized porous silicon-solid lipid nanocomposites (THCPSi-SLNCs) on a ratio 1:1 prepared by the solid-in-oil-in-water emulsion solvent evaporation method are produced in order to enhance the suspensibility of the nanoparticles and the stability against aggregation in aqueous buffer solutions, as well as to increase the particle surface smoothness and cytocompatibility, reduce the particle's cellular association, increase the in vitro stability in human plasma, and prolong the loaded drug release.

#### **FULL PAPERS**

Mixed metal-semiconductor nanocrystal aerogels, which are light-emitting and highly porous macroscopic monoliths, are fabricated. Thiol-stabilized CdTe and Au nanoparticles from aqueous synthesis act as building blocks. The content and the properties of the aerogels are tuned by variation of the initial CdTe to Au nanoparticle ratio. Materials of this type combining the optical and catalytic properties of their nanoscale building blocks with very high porosity of the gel structure are of special interest for applications in nanosensing and photocatalysis.

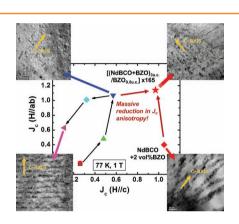


#### **Semiconductors**

T. Hendel, V. Lesnyak, L. Kühn, A.-K. Herrmann, N. C. Bigall, L. Borchardt, S. Kaskel, N. Gaponik, A. Eychmüller\*......1903–1911

Mixed Aerogels from Au and CdTe Nanoparticles

Spontaneous self-assembly of a multication nanophase in another multication matrix phase is a promising bottom-up approach to fabricate novel, nanocomposite structures for a range of applications. The first complimentary experimental and theoretical studies are reported to first understand and then control or guide the self-assembly of insulating BaZrO<sub>2</sub> nanodots within REBa<sub>2</sub>Cu<sub>3</sub>O<sub>7- $\delta$ </sub> (RE = rare earth elements including Y, REBCO) superconducting films. The results have broad implications for fabrication of controlled selfassembled nanostructures for a range of applications via strain-tuning.

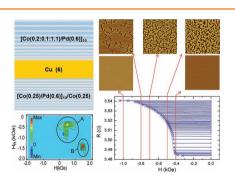


#### **Self-Assembly**

S. H. Wee, Y. Gao, Y. L. Zuev, K. L. More, J. Meng, J. Zhong, G. M. Stocks, A. Goyal\* .......1912–1918

Self-Assembly of Nanostructured, Complex, Multication Films via Spontaneous Phase Separation and Strain-Driven Ordering

A virtually continuous range of resistance states is demonstrated in graded anisotropy pseudo spin valves. An analysis of first-order reversal curves combined with magnetic force microscopy shows that the origin of the effect is the field-dependent population of up and down domains in the free layer.

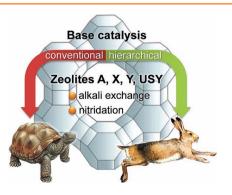


#### **Spintronics**

Y. Fang, R. K. Dumas, T. N. A. Nguyen, S. M. Mohseni, S. Chung, C. W. Miller, J. Åkerman\*......1919–1922

A Nonvolatile Spintronic Memory Element with a Continuum of Resistance States

Hierarchical FAU and LTA-type zeolites are prepared through post-synthetic strategies and display exceptional performance in base catalysis. A thorough characterization demonstrates that the presence of a secondary level of mesoporosity facilitates the introduction of base functionality by alkali ion exchange or nitridation in ammonia. The enhanced activity in the Knoevenagel condensation of benzaldehyde with malononitrile emphasizes that, in the design of basic zeolite catalysts, auxiliary porosity plays a key role.



#### **Catalysis**

D. Verboekend, T. C. Keller, S. Mitchell, J. Pérez-Ramírez\*......1923–1934

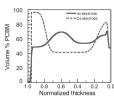
Hierarchical FAU- and LTA-Type Zeolites by Post-Synthetic Design: A New Generation of Highly Efficient Base Catalysts

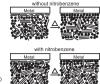
#### **FULL PAPERS**

#### **Photovoltaic Devices**

S. A. Mauger, L. Chang, S. Friedrich, C. W. Rochester, D. M. Huang, P. Wang, A. J. Moulé\*........1935–1946

Self-Assembly of Selective Interfaces in Organic Photovoltaics



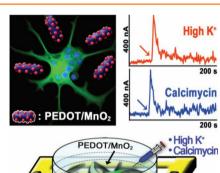


It is shown that the metal capping electrode in an organic photovoltaic device affects the stratification of materials in the bulk heterojunction (BHJ) and that solvent additives can inhibit stratification. It is found that some metals can donate charge to (6,6)-phenyl-C<sub>61</sub>-butyric acid methyl ester (PCBM). The enrichment and charging of PCBM at the interface with the metal increases device power conversion efficiency.

#### **Bioelectronics**

S. Kim, W.-K. Oh, Y. S. Jeong, J. Jang\*.....1947–1956

Dual-Functional Poly(3,4ethylenedioxythiophene)/MnO<sub>2</sub> Nanoellipsoids for Enhancement of Neurite Outgrowth and Exocytosed Biomolecule Sensing in PC12 Cells



A poly(3,4-ethylenedioxythiophene) (PED-OT)/MnO<sub>2</sub> nanoellipsoid is fabricated for facilitating the neurite outgrowth during differentiation and detecting exocytized biomolecules from PC12 cells. PC12 cells co-incubated with PEDOT/MnO<sub>2</sub> nanoellipsoids and nerve growth factor demonstrate enhanced neurite outgrowth. Exocytosis of catecholamines is electrically detected by a PEDOT/MnO<sub>2</sub> nanoellipsoid sensor.

## Thin Films

B. Scherrer,\* M. V. F. Schlupp,

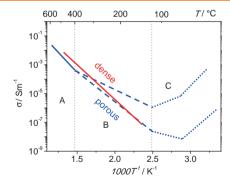
D. Stender, J. Martynczuk,

J. G. Grolig, H. Ma, P. Kocher,

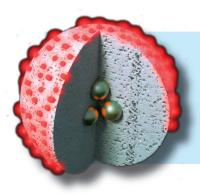
T. Lippert, M. Prestat,

L. J. Gauckler ......1957-1964

On Proton Conductivity in Porous and Dense Yttria Stabilized Zirconia at Low Temperature



The electrical conductivity below 400 °C of porous yttria stabilized zirconia (YSZ) deviates from the oxygen-ion conductivity due to proton conduction via chemisorbed water in the form of hydroxyl groups at the inner surface. Below 120 °C, proton conductivity via physisorbed water in the nanoporous microstructures sets in (Grotthuss mechanism). Dense thin films show oxygen-ion conductivity only and no proton conductivity is present.



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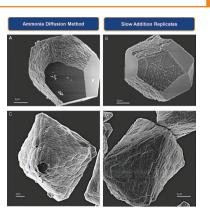
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Elucidation of the changes in solution that accompany CaCO<sub>3</sub> precipitation by the widely used ammonia diffusion method enables replication of calcite mesocrystals via a simple and highly reproducible titration-based method. The experiments also demonstrate that aggregation-based growth, which generates these complex structures, is promoted by high and constant supersaturation levels, giving insight into the mechanisms of mesocrystal formation.



### **FULL PAPER**

#### Crystallization

J. Ihli,\* P. Bots, A. Kulak, L. G. Benning, F. C. Meldrum\*.....1965–1973

Elucidating Mechanisms of Diffusion-**Based Calcium Carbonate Synthesis** Leads to Controlled Mesocrystal **Formation** 

1863