

mers. One of the polymers (an indenofluorene analogue of F8BT) shows no photovoltaic activity, while the other achieves reasonable power conversion efficiencies of up to 1.9%. The photoluminescence spectrum of the ineffective blend shows emission from a PCBM singlet exciton which is not present for

the latter superior polymer and suggests that energy transfer to the acceptor material is taking place. Given the strong photoluminescence from this polymer and its larger degree of overlap with the absorption spectrum of PCBM, there should indeed be fast Förster resonant energy transfer

PCBM exciton which, instead of generating a current, either relaxes to the ground state or crosses to a triplet state. A photocurrent could nonetheless be generated from this process if, in reverse fashion, the hole generated in the highest occupied molecular orbital (HOMO) of the PCBM were to hop to the HOMO of the polymer. For this polymer it seems that there is not enough energy remaining in the PCBM exciton to drive this process, but it is likely that hole transfer is responsible for photocurrents generated in other polymers which show strong photoluminescence toward the blue end of the spectrum.

The research goes a long way toward explaining the difficulties of using intensely photoluminescent polymers in organic solar cells and provides an important clue for designing photovoltaics that absorb blue light. Polymers for this purpose would benefit from having weakly emissive excitons that do not favor the wasteful energy transfer.

Tobias Lockwood

between the two materials.

For a photocurrent to be generated in the blend, an electron excited in the polymer has to be transferred to the PCBM and from there to an electrode. In the poorly performing poly-indenofluorene this process is slow compared to a transfer of the electron's energy to create a

Nano Focus

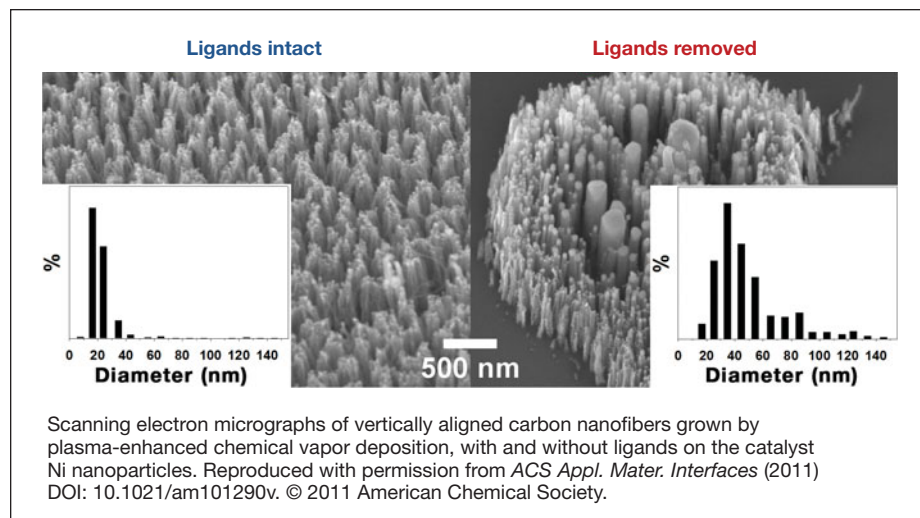
Organic ligands encapsulating catalytic nanoparticles improve monodispersity of vertically aligned carbon nanofibers

Regular arrays of vertically-aligned carbon nanofibers are actively sought: Due to their anisotropy and high surface area-to-volume ratio, they could be useful in many areas in nanotechnology. They can be grown from catalyst nanoparticles deposited on a substrate. Fibers with monodisperse diameters above 100 nm can be grown from dewetted catalyst thin films. For diameters below 100 nm, electron beam lithography is very successful, but the cost of this technique is an obstacle for commercialization. Alternatively, for these sizes, chemically synthesized nanoparticles can be used as seeds for nanofiber growth. M.F. Sarac, R.M. Wilson, A.V. Melechko, J.B. Tracy from North Carolina State University, K.L. Klein from the National Institute of Standards

and Technology, and their colleagues show the influence of the ligands capping Ni catalyst nanoparticles for obtaining monodisperse, regular arrays of vertically-aligned nanofibers with diameters up to 100 nm.

As reported in the March 16th online edition of *ACS Applied Materials & Interfaces* (DOI: 10.1021/am101290v),

the researchers compared nanofibers grown by plasma-enhanced chemical vapor deposition. The seeds were Ni catalyst nanoparticles, either capped by organic ligands (trioctylphosphine and oleylamine), or after ligand removal with UV-ozone treatment. The fibers obtained from ligand-capped nanoparticles are monodisperse of diameter and



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June 30, 2011

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more regularly spaced, whereas the ones obtained from nanoparticles without ligands have a larger mean diameter and a broad dispersion of diameters. The UV-ozone treatment itself leaves the Ni nanoparticle core sizes unchanged, but during heating to 700°C, particles without ligands agglomerate and coalesce,

which results in polydisperse seeds for nanofiber growth. Coalescence occurs only prior to nanofiber growth: Once growth is initiated, no further coalescence can occur, and the fibers grow separately.

The researchers have also demonstrated the formation of graphitic shells

around the ligand-capped particles during the pre-growth heating. The shells are made of the carbon atoms from the ligand molecules. They protect the particles from agglomeration and also serve as a carbon source for the initial stage of carbon nanofiber growth.

Elsa Couderc

Nano Focus

Self-cooling observed in graphene electronics

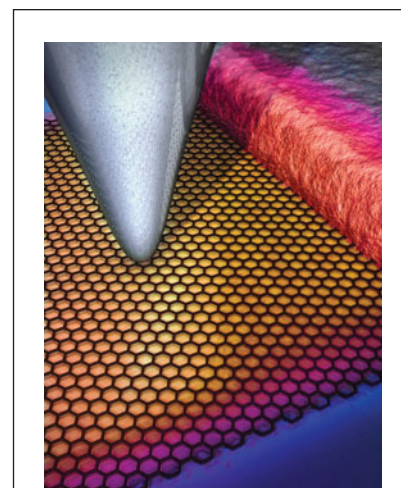
Cooling electronic devices such as computers consumes a great deal of energy, typically in the form of air or water cooling. But what if the materials used in making the electronics cooled themselves during operation? Recent findings by William King and Eric Pop of the University of Illinois, Urbana-Champaign, published April 3rd in the online journal *Nature Nanotechnology* (DOI: 10.1038/nnano.2011.39), suggest that graphene components may be able to do just that.

Using a method they developed to measure the nanoscale temperature distribution with atomic force microscopy (AFM) tips, they were able to determine the temperature distribution in a working graphene field-effect transistor (FET) with a spatial resolution of about 10 nm and a thermal resolution of about 0.25°C. They used this data to construct tempera-

ture maps of the FET. “The first thing that was remarkable to me,” King said, “was that we could actually measure the temperature of a working FET where the device layer was just 1 atom thick.”

By feeding temperature data from these maps into a simulation program developed by Pop, they discovered that the temperature rise at a graphene/metal junction in the circuit differed depending on the direction of current flow through the device. In fact, they found a thermoelectric “nanoscale cooling” effect that accounted for about one-third of the temperature difference; the rest was due to resistive heating.

Additional simulations that looked at possible future improvements in graphene materials and metal contacts showed further promise for self-cooling electronics. “If graphene improves in the way that everyone thinks it will, the thermoelectric effect will grow in importance, and the resistive heating will shrink,” King said. “Projecting forward to carbon electronics of the future, the



An atomic force microscope tip scans the surface of a graphene/metal contact to measure temperature with spatial resolution of about 10 nm and temperature resolution of about 250 mK. Color represents temperature data. Credit: Alex Jerez, Beckman Institute Imaging Technology Group

thermoelectric cooling effect will govern everything about the contacts.”

Tim Palucka

Computational method used to construct database of new zeolite-like materials

Industrial applications for zeolites include catalysis, ion exchange, and separations. The scope of applicability would increase with the discovery of new zeolites (currently fewer than 200 zeolites are known), which can be stimulated with computational predictions of stable, zeolite-like structures. Recently, R.S. Pophale and M.W. Deem of Rice University, in collaboration with

P.A. Cheeseman of Purdue University, refined their previously published computational approach by accounting for the Pauli exclusion principle, and constructed a database of predicted, zeolite-like materials.

As reported recently in the online edition of *Physical Chemistry Chemical Physics* (DOI: 10.1039/c0cp02255a), Pophale, Cheeseman, and Deem developed a Monte Carlo technique to randomly sample the structural space of low-energy, zeolite-like structures. Geometry optimizations were performed with two interatomic potentials—the Sanders-

Leslie-Catlow potential, which is accurate for zeolites, and the van Beest-Kramer-van Santen potential, which agrees well with experimentally determined enthalpies of formation. Enforcing the Pauli exclusion principle makes the structures resulting from the two potentials much more realistic, stable, and similar to each other.

Over 2.6 M zeolite-like structures were found and about 10% have energies in the range of known zeolites. Calculated powder x-ray diffraction patterns for the database structures are similar to those of known zeolites.