



Energy Focus

Nanocomposites improve performance of electrode materials for Li-ion batteries

Researchers J. Xiao, J.P. Lemmon, and collaborators at Pacific Northwest National Laboratory picked up an old recipe and found out something new. The group synthesized nanocomposites of exfoliated MoS₂ and polyethylene oxide (PEO) using an existing technique. This time, however, they electrochemically tested the composite as a negative electrode in Li-ion batteries. In the August 24th issue of *Chemistry of Materials* (DOI:10.1021/cm101254j; p. 4522), the researchers report that the nanocomposite with 5 wt% PEO revealed very high specific capacity (reaching 1131 mAh/g) and longer cycle life than MoS₂ alone. Graphite, a conventional negative electrode battery material, has a theoretical capacity of 372 mAh/g.

MoS₂ is a promising alternative electrode material because it forms layers that are loosely coupled by weak van der Waals interactions, and the Li⁺ ions can diffuse in the layers without inducing large volume change. The researchers

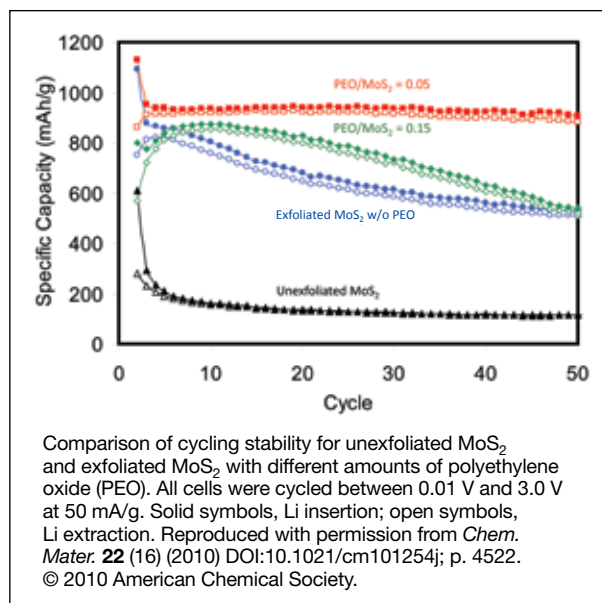
found by scanning electron microscopy that exfoliated MoS₂ with weight percents of 0, 5, and 15 PEO exhibits a layered morphology with the morphology becoming more distinct with increasing polymer addition. The x-ray diffraction data and high-resolution transmission electron microscopy (HRTEM) images of the 5 wt% PEO material showed that the polymer does not significantly affect the *d*-spacing of exfoliated MoS₂ in the composite, but a weak reflection in the x-ray diffraction data of the 15 wt% PEO material suggests that as more PEO is added, a more ordered composite phase begins to form.

The researchers conclude that the very high capacity and cycling stability of 5 wt% PEO/MoS₂ is due to PEO maintaining a disorder in MoS₂ that allows Li⁺ ions to diffuse into and out of the material repeatedly during cycling. PEO also coats the nanocomposite particles, which may

enhance the ionic diffusion between electrolyte and particles.

The HRTEM micrographs showed that pristine, unexfoliated MoS₂ existed with the PEO/MoS₂ nanocomposite in the samples of prepared material. This finding “suggest[s] that it is possible to further improve the capacity of the composite by further optimizing the synthesis condition.”

Ashley Predith



Energy Focus

Improved light emission in Ce³⁺ and Tb³⁺ co-doped MgY₄Si₃O₁₃ phosphors

White light-emitting diodes (LEDs) have recently been investigated to be employed in solid-state lighting device applications. A widely utilized approach to producing white LEDs is to combine blue LEDs with yellow-emitting phosphors (YAG: Ce³⁺). Consequently, these LEDs produce cool white emissions and a low color rendering index due to their weak emissions in the green and red spectral range. An alternate approach for white lighting applications uses tri-color (red, green, and blue)-emitting phosphors excited by ultraviolet (UV) LEDs. Conventional phosphors are not suitable for white light-emitting systems employing UV-LEDs due to their weak

absorption in the near-UV (NUV) region. Now, H.-Y. Chung, C.-H. Lu, and C.-H. Hsu of National Taiwan University have made strides toward overcoming these obstacles in solid-state lighting.

In the July issue of the *Journal of the American Ceramic Society* (DOI: 10.1111/j.1551-2916.2010.03626.x; p. 1838), the research team reported the synthesis and luminescence properties of MgY₄Si₃O₁₃-based phosphors, co-doped with varying concentrations of Ce³⁺ and Tb³⁺. The Mg(Y_{4-x-y}Ce_xTb_y)Si₃O₁₃, (0 ≤ x ≤ 0.2, 0 ≤ y ≤ 1.0) were prepared through a solid-state route, by grinding MgO, Y₂O₃, CeO₂, Tb₄O₇, and SiO₂ in a ball mill. Mixed powders were heated at 1400°C for 4 h in a tubular furnace under a reducing atmosphere (5 vol% H₂ and 95 vol% N₂).

The research team observed a marked enhancement in emission intensity from

the co-doped samples, which was expected to be the effect of energy transfer between Ce³⁺ and Tb³⁺. The excitation spectra appeared to result from the sensitizer Ce³⁺ and the line emission spectra originated from the activator Tb³⁺. By comparing emissions of Mg(Y_{3.6}Ce_{0.2}Tb_{0.2})Si₃O₁₃ and Mg(Y_{3.8}Tb_{0.2})Si₃O₁₃, the emission intensity at 544 nm of the co-doped sample was 20 times that of the sample doped only with Tb³⁺.

Similarly, the highest quantum efficiency of 49% observed in Mg(Y_{3.4}Ce_{0.2}Tb_{0.4})Si₃O₁₃ was increased from the 37% efficiency in Mg(Y_{3.8}Ce_{0.2})Si₃O₁₃, which was void of Tb³⁺. However, for y > 0.4, a decrease in emission intensity is observed as the result of concentration quenching. With an increase in activator ions, the researchers observed increased interaction between

neighboring Tb^{3+} resulting in a reduction in luminescence.

In addition, the emitting color varied from bluish-green to greenish-yellow

with increasing Tb^{3+} content. Excited at 330 nm, the Commission Internationale de l'Éclairage (CIE) chromaticity coordinates shifted from (0.25, 0.33) to

(0.40, 0.52) as the value of y increased from 0.1 to 0.6 in the $Mg(Y_{3.8-y}Ce_{0.2}Tb_y)Si_3O_{13}$ materials.

Melissa A. Harrison

Energy Focus

Quantum efficiency improved in bulk heterojunction PVs

Although bulk heterojunction photovoltaics (BHJs) are attractive as low-cost solar cells due to their ease of processability, devices incorporating low-bandgap quantum dots (QDs) fall short of the performance achieved by analogous blends of polymers and CdSe QDs. Previously, D.S. Ginger, S.A. Jenekhe, and co-researchers at the University of Washington, Seattle, hypothesized that the poor performance by BHJs composed of PbS QDs blended with common conjugated polymers is due to insufficient photoinduced charge transfer at the organic–inorganic interface. Recently, Ginger and co-researchers showed that BHJs made from PbS QDs and new donor–acceptor polymers exhibit efficiencies two orders of magnitude greater than those observed for blends of PbS with conventional host polymers.

As reported in the July 14th issue of *Nano Letters* (DOI: 10.1021/nl1013663; p. 2635), Ginger and co-researchers selected three polymers (PDTPQx, PDTPPPz, and PDTPBT; see figure) to blend with PbS QDs because their ionization potentials show that their highest occupied molecular orbitals lie within the PbS bandgap. Photoinduced absorption (PIA) spectroscopy shows that in the

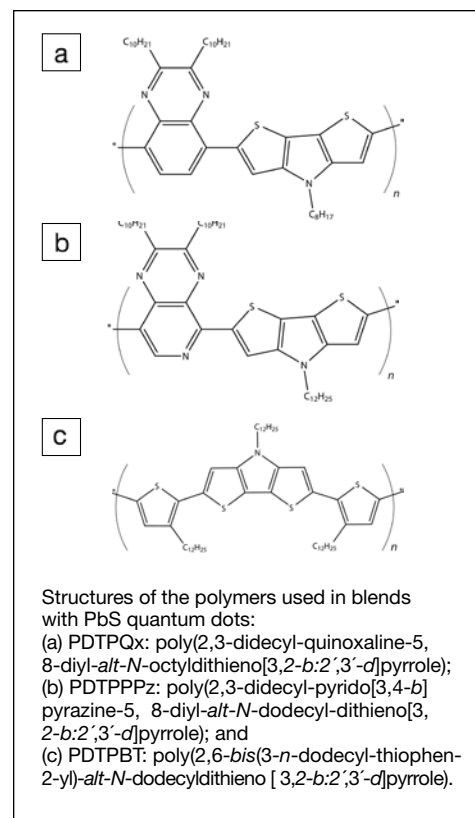
range of 0.8 eV to 2.2 eV BHJ blends of PDTPQx and PbS QDs exhibit new sub-bandgap absorptions by the PDTPQx and a bleach of the polymer's bandgap transition following photoexcitation, while the PDTPBT blend shows very weak PIA signal, and the PDTPPPz blend shows no detectable PIA signals. Because neat PDTPQx shows no PIA signal, the researchers attribute the blend's PIA spectrum to long-lived polarons on the PDTPQx polymer chains created by photoinduced electron transfer from the polymer to the PbS QDs, leading them to predict PDTPQx/PbS to perform significantly better in BHJ photodiodes than PbS QDs blended with either of the other two polymers considered. The researchers verified this prediction by showing that the quantum efficiencies exhibited by the PDTPQx/PbS blends are two orders of magnitude higher than those exhibited by blends with the other two polymers.

Under simulated AM 1.5 illumination, the researchers estimated a power conversion efficiency (PCE) of about 0.55%, which is modest in comparison to polymer-fullerene BHJ cells but is significantly higher than BHJ devices made from previous polymer blends with low-bandgap QDs. The researchers plan to improve performance by increasing the PDTPQx molecular weight to facilitate thicker films, and by controlling the shape of the QDs.

The researchers said, “We anticipate

that the viability of new organic host materials when blended with PbS should reinvigorate the study of solution-processable bulk-heterojunction excitonic solar cells made with a range of low-bandgap nanoparticles and should facilitate their use in both hybrid photovoltaics and photodetectors with bandgaps tailored via quantum confinement.”

Steven Trohalaki



Normal modes and density of states achieved in disordered colloidal solids

Colloidal suspensions have been used as model systems in experimental research on the fundamentals of statistical mechanics. In colloidal systems,

a crystal or amorphous structural glass can be produced using traditional hard-sphere particles such as silica sphere. However, the perfect crystals produced with these conventional particles show spatial homogeneous fluctuations. These fluctuations are measured using optical microscopy to observe individual particle motion within the interior of the system.

Recently, D. Kaya, N.L. Green, C.E. Maloney, and M.F. Islam of Carnegie Mellon University developed an approach to measure the correlation in particle displacement using strongly disordered colloidal crystals composed of deformable microgel colloidal particles to determine the normal modes and the density of states (DOS). Normal modes and the DOS of a