Enabling Nanoscience: From Computation to Experimental Assay Tools

One unique aspect of nanostructured materials is the diversity of morphologies that can be achieved using various building blocks and processing techniques, including nanolayered two-dimensional assemblies, complex interconnected networks, and nanoporous structures. When nanoscale assembly and materials are used to combine different functional materials systems, unique enhancements of properties can be achieved, but these properties are often difficult to predict. This observation is particularly relevant to the construction of organic and organic−inorganic hybrid solar materials, for which the tuning of carrier transport, control of materials interfaces, and ability to maintain charge separation over nanometer-scale distances becomes key to improving device efficiencies;[1−3] a major challenge faced in the extension of nanomaterials to solar applications is the ability to predict the effects that material morphology and architecture will have in final device performance. In this issue, Fan Yang and Stephen Forrest of the University of Michigan demonstrate the power of molecular-scale dynamics simulations to predict the photocurrent generation and transport properties in organic solar cells devised with a broad range of different morphologies.[4] By utilizing dynamics simulations in conjunction with available experimental data, the authors are able to calculate actual power conversion efficiencies and provide optimal thicknesses for each morphology. The ability to connect known data with a realistic model offers a meaningful roadmap for materials scientists and engineers who design nanostructured photovoltaics, regardless of material type. This paper is an elegant example of the power of simulation and molecular modeling in guiding nanostructured materials synthesis and assembly for highly desired properties.[5]

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Consistent with the theme of nanomaterials as diverse systems is the challenge of measuring critical properties or characteristics of such systems, particularly when a large number of variations of a material set must be probed over reasonable experimental time scales. This capability becomes even more significant when one addresses issues that impact human health, such as the biocompatibility and toxicity of the many new and exciting nanomaterials systems currently being developed for drug delivery, gene and siRNA delivery, and bio-imaging, examples of which have recently been featured in this journal.[6−10] With the development of each new nanomaterial designed for direct introduction into the bloodstream or accumulation in tissues of the body, there are potential concerns and questions that must be addressed to ensure the health of the patient. The ability to functionalize the surfaces of many nanoparticles with organic or inorganic exterior layers, as well as differences in synthetic routes, charge density, and particle size, are factors that increase the number of tests that could be required of even a relatively simple nanoparticle system to achieve optimal biocompatibility. Nick Kotov of the University of Michigan, Yurii Gun'ko of Trinity College Dublin, and their co-workers present a new way to address this problem with a rapid, high-content screening assay that enables the testing of large panels of nanoparticles.[11] Using an approach that enables the analyses of up to 25 000 individual cells in one experiment, they show that it is possible to achieve a far more complete picture of the impact of different nanomaterials by extending methods that primarily focused on cell death

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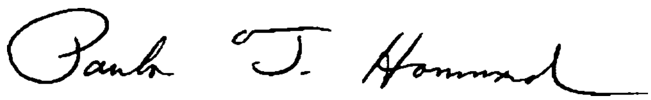
to include a number of intracellular activities and functions. The ability to examine subtle changes in cellular behavior and function on the single-cell level provides a highly refined tool for predicting the impact of nanoparticles on various tissues, allowing one to infer the nature of cell–nanoparticle interactions in a way that would not be possible using traditional methods. Furthering approaches such as this will enable the development of nanotoxicity databases and advance the implementation of nanomaterials in medicine.



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