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## ARTIFICIAL INTELLIGENCE PROSPECTIVE

### Growing field of materials informatics: Databases and artificial intelligence

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The paradigm of molecular discovery in the chemical and pharmaceutical industry has followed a repetitive succession of screening and synthesis, involving the analysis of individual molecules that were both natural and produced. This ability to generate and screen libraries of compounds has found an echo in solid-state physics with the demand to explore and produce new materials for testing. In response to this demand, a golden age of materials discovery is being developed, with progress on important areas of both basic science and device applications. The confluence of theoretical and simulation methods, together with the availability of computation resources, has established the "materials genome" approach that is used by a growing number of research groups around the world with the goal of innovating on materials through systematic discovery. The authors provide an overview of this group of methodologies in tackling the ever-increasing complexity of computational materials science simulations. Computational simulation is highlighted as a major component of rational design and synthesis of new materials with targeted properties, describing progress on databases and large data treatment. Tools for new materials discovery, including progress on the deployment of new data repositories, the implementation of high-throughput simulation approaches, and the development of artificial intelligence algorithms, are discussed. doi.org/10.1557/mrc.2020.2

## PROSPECTIVES

### A perspective on overcoming water-related stability challenges in molecular and hybrid semiconductors

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Molecular semiconductors synergize a variety of uniquely advantageous properties such as excellent absorption and emission properties, soft and deformable mechanical properties, and mixed ionic and electrical conduction. Over the past two decades, this outstanding set of features has put molecular semiconductors in the spotlight for a variety of optoelectronics and sensing applications. When it comes to mass-market adaptation, however, a challenge in these soft and van der Waals-bonded materials remains their electrical as well as environmental stability and degradation. The authors summarize their current understanding of why organic semiconductors degrade with a strong emphasis placed on the quintessential role played by water in this process. Furthermore, it will be revisited by which mechanisms water-related stability shortcomings might be addressed in the future, and how these lessons can be translated to relevant hybrid systems such as perovskites and carbon nanotubes. Throughout this discussion, some parallels and key differences between organic and hybrid materials will be highlighted, and it will be elaborated on how this affects the associated device stability. doi.org/10.1557/mrc.2019.161

### Planet–satellite nanostructures from inorganic nanoparticles: From synthesis to emerging applications

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Planet–satellite-type supracolloidal clusters represent a comparably young class of nanomaterials, which are unique with regard to structural order. Different approaches for their synthesis are discussed and compared. These synthetic methods enable the engineering of supracolloidal structural and adaptive properties, which in turn enables different emerging applications, such as in sensing and catalysis. These possibilities are explored on the basis of selected recent examples. A perspective about possible future developments is given at the end of this prospective. doi.org/10.1557/mrc.2019.163

## ARTICLES

### Deep learning-based super-resolution for small-angle neutron-scattering data: Attempt to accelerate experimental workflow

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The authors propose an alternative route to circumvent the limitation of neutron flux using the recent deep learning super-resolution technique. The feasibility of accelerating data collection has been demonstrated by using small-angle neutron-scattering (SANS) data collected from the EQ-SANS instrument at the Spallation Neutron Source (SNS). Data collection time can be reduced by increasing the size of binning of the detector pixels at the sacrifice of resolution. High-resolution scattering data are then reconstructed by using a deep learning-based super-resolution method. This will allow users to make critical decisions at a much earlier stage of data collection, which can accelerate the overall experimental workflow. doi.org/10.1557/mrc.2019.166

### Design space visualization for guiding investments in biodegradable and sustainably sourced materials

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In many materials development projects, scientists and research heads make decisions to guide the project direction. For example, scientists may decide which processing steps to use, what elements to include in their materials selection, or from what suppliers to source their materials. Research heads may decide whether to invest development efforts in reducing the environmental impact or production cost of a material. When making these decisions, it would be helpful to know how those decisions affect the achievable performance of the materials under consideration. Often, these decisions are complicated by tradeoffs in performance between competing properties. The authors present an approach for visualizing and evaluating design spaces, where a design space is defined as the set of possible materials under consideration given specified constraints. This design space visualization approach is applied to two case studies with environmental impact motivations: one in biodegradability for solvents, and the other in sustainable materials sourcing for Li-ion batteries. The results demonstrate how this visualization approach can enable data-driven, quantitative decisions for project direction. doi.org/10.1557/mrc.2020.5

### Highly stable multilayered silicon-intercalated graphene anodes for Li-ion batteries

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To avoid degradation of silicon anodes in lithium-ion batteries (LIBs), the authors report a new two-dimensional multilayered Si-intercalated rGO (rGO/Si) anode prepared by direct growth of Si into a porous multilayered reduced graphene oxide (rGO) film. Direct Si deposition onto the porous rGO film allows the Si layers to be intercalated into the film via *in situ* replacement of the oxygen groups of the multilayered graphene oxide (GO) with Si through thermal reduction of the GO film. The porous rGO acts as a cushion against the expansion of the Si layer during lithiation, preventing the Si from being pulverized and producing highly stable LIBs. doi.org/10.1557/mrc.2020.14

## Loss in acoustic metasurfaces: A blessing in disguise

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From being an unfavorable consequence to finding itself as the intended imaginary part of a non-Hermitian system, loss has truly emerged as more of a friend than a foe in the context of acoustic metasurfaces. With the promising features of sub-wavelength geometries and the rapid advances in manufacturing techniques that can enable their realization, loss becomes a central topic of discussion. Further, the capability of introducing and tailoring loss allows it to serve as a new degree of freedom in passive wavefront shaping devices. In this review, the authors look back at the recent progress in the field of lossy acoustic metasurfaces. The background behind loss in deep subwavelength geometries and the instinctive responses to treat them and exploit them are overviewed, followed by more recent works that embrace and tailor their behavior for unconventional applications. The forthcoming years for acoustic metasurfaces thus hold several promising avenues for exploration, with loss as the protagonist. doi.org/10.1557/mrc.2019.148

## Mechanical and failure behaviors of lattice-plate hybrid structures

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The authors design six alumina hybrid structures consisting of stretching-dominated plates and different space-filling lattices comprised of hollow tubes and perform finite element simulations to study mechanical and failure behaviors of such hybrid structures. They investigate the effects of three geometrical parameters on the stiffness and failure of these hybrid structures and further compare their advantages and disadvantages. The authors find that the failure modes of these hybrid structures can be tuned by altering cell unit type and geometrical parameters. Among these hybrid structures, the ones with effective support from the lattice unit cells in the stretching direction exhibit better specific stiffness and strength. By varying the lattice and plate thickness, the authors find that the relationship between stiffness/failure strength and density follow a power law. When intrinsic material failure occurs, the power law exponent is 1; when buckling failure arises, the power law exponent is 3. However, by varying tube thickness, the relationship follows an unusual power law with the exponent changing from nearly 0 to nearly infinity. In addition, the hybrid structures also exhibit defect insensitivity. This study shows that such hybrid structures are able to greatly expand the design space of architectured cellular materials for engineering applications. doi.org/10.1557/mrc.2019.153

## The role of Toll-like receptor signaling in the macrophage response to implanted materials

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Inflammation is facilitated largely by macrophages and other white blood cells, which recognize and respond to evolutionarily conserved damage-associated molecular patterns that are released upon tissue injury and cell stress. Damage-associated molecular patterns are known to bind Toll-like receptors (TLRs) and initiate inflammatory responses through MyD88-dependent NF-κB signaling. Biomaterial implantation activates the innate immune system, resulting in a chronic inflammatory response known as a foreign body reaction (FBR). The authors discuss the current understanding of damage-initiated TLR signaling in the FBR and the significance of this response in the success of implanted devices. doi.org/10.1557/mrc.2019.154

## Multilayer multifunctional advanced coatings for receivers of concentrated solar power plants

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The extending market of concentrated solar power plants requires high-temperature materials for solar surface receivers that would ideally heat an air coolant beyond 1300 K. The authors present an investigation on high-temperature alloys with ceramic coatings (AlN or SiC/AlN stacking) to combine the properties of the substrate (creep resistance, machinability) and coating (slow oxidation kinetics, high solar absorptivity). The first results showed that high-temperature oxidation resistance and optical properties of metallic alloys were improved by the different coatings. However, the fast thermal shocks led to high stress levels not compatible due to the differences in the coefficient of thermal expansion. doi.org/10.1557/mrc.2019.130

## Response of neuroglia to hypoxia-induced oxidative stress using enzymatically cross-linked hydrogels

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Three-dimensional cultures have exciting potential to mimic aspects of healthy and diseased brain tissue to examine the role of physiological conditions on neural biomarkers, as well as disease onset and progression. Hypoxia is associated with oxidative stress, mitochondrial damage, and inflammation, key processes potentially involved in Alzheimer's and multiple sclerosis. The authors describe the use of an enzymatically cross-linkable gelatin hydrogel system within a microfluidic device to explore the effects of hypoxia-induced oxidative stress on rat neuroglia, human astrocyte reactivity, and myelin production. This versatile platform offers new possibilities for drug discovery and modeling disease progression. doi.org/10.1557/mrc.2019.159

## Electronic charge-transfer properties of COF-5 solutions and films with intercalated metal ions

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To investigate the manipulation of electromagnetic properties of two-dimensional materials, this effort characterizes charge-transfer behavior of colloidal COF-5 (covalent organic framework) in the presence of various metal ions. A series of metal chloride compounds was introduced to COF-5 in solution and solid film phases, and the interaction of the material with electromagnetic radiation was monitored across the visible region using electronic absorption spectroscopy. Notable changes were observed, quantified, and discussed for copper (II) chloride ($CuCl_2$), chromium (III) chloride ($CrCl_3$), and iron (III) chloride ($FeCl_3$) with COF-5. Ligand-to-metal and metal-to-ligand charge transfer are explored as a possible mechanism for the observed electronic behaviors. doi.org/10.1557/mrc.2020.7



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