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ARTIFICIAL INTELLIGENCE SPECIAL ISSUE: RESEARCH LETTERS

A picture is worth a thousand words: Applying natural language processing tools for creating a quantum materials database map

Vineeth Venugopal, **Scott R. Broderick**, **Krishna Rajan**, University at Buffalo, The State University of New York, USA

The authors demonstrate the application of natural language processing (NLP) tools to explore large libraries of documents and to correlate heuristic associations between text descriptions in figure captions with interpretations of images and figures. The use of visualization tools based on NLP methods permits one to quickly assess the extent of the research described in the literature related to a specific topic. The authors demonstrate how the use of NLP methods on only the figure captions without having to navigate the entire text of a document can provide an accelerated assessment of the literature in a given domain. doi.org/10.1557/mrc.2019.136

A data ecosystem to support machine learning in materials science

Ben Blaiszik, **Logan Ward**, The University of Chicago, and Argonne National Laboratory, USA; **Marcus Schwarting**, Argonne National Laboratory, USA; **Jonathon Gaff**, The University of Chicago, USA; **Ryan Chard**, The University of Chicago, and Argonne National Laboratory, USA; **Daniel Pike**, Cornell University; **Kyle Chard**, **Ian Foster**, The University of Chicago, and Argonne National Laboratory, USA

Facilitating the application of machine learning (ML) to materials science problems requires enhancing the data ecosystem to enable discovery and collection of data from many sources, automated dissemination of new data across the ecosystem, and the connecting of data with materials-specific ML models. Here, we present two projects, the Materials Data Facility (MDF) and the Data and Learning Hub for Science (DLHub), that address these needs. We use examples to show how MDF and DLHub capabilities can be leveraged to link data with ML models and how users can access those capabilities through web and programmatic interfaces. doi.org/10.1557/mrc.2019.118

PROSPECTIVES

Theory and simulations of critical temperatures in CrI_3 and other 2D materials: Easy-axis magnetic order and easy-plane Kosterlitz–Thouless transitions

Thomas Olsen, Technical University of Denmark, Denmark

The recent observations of ferromagnetic order in several two-dimensional (2D) materials have generated an enormous interest in the physical mechanisms underlying 2D magnetism. In the present prospective prticle, the author shows that density functional theory combined with either classical Monte Carlo simulations or renormalized spin-wave theory can predict Curie temperatures for ferromagnetic insulators that are in quantitative agreement with experiments. The case of materials with in-plane anisotropy is then discussed, and it is argued that finite size effects may lead to observable magnetic order in macroscopic samples even if long-range magnetic order is forbidden by the Mermin–Wagner theorem. doi.org/10.1557/mrc.2019.117

Redox-active polymers (redoxmers) for electrochemical energy storage

Mengxi Yang, **Kewei Liu**, **Ilya A. Shkrob**, **Chen Liao**, Argonne National Laboratory, USA

Polymer redox-active materials (redoxmers) have numerous applications in the emerging electrochemical energy-storage systems due to their structural versatility, fast-cycling ability, high theoretical capacity as electrode materials, sustainability, and recyclability. The authors examine recent developments in improving the cycling performance of such materials and provide a vista on future research directions. doi.org/10.1557/mrc.2019.122

Three-dimensional printed molds and materials for injection molding and rapid tooling applications

John Ryan C. Dizon, Case Western Reserve University, USA, and Bataan Peninsula State University, Philippines; **Arnaldo D. Valino**, Case Western Reserve University, USA, and Adamson University, Philippines; **Lucio R. Souza**, Case Western Reserve University, USA; **Alejandro H. Espera**, Case Western Reserve University, USA, Ateneo de Davao University, Philippines, and Virginia Tech, USA; **Qiyi Chen**, **Rigoberto C. Advincula**, Case Western Reserve University, USA

The authors cover an overview of the injection molding process and the importance of mold design and tooling considerations, important material requirements and thermal properties for molds, polymer material requirements for injection molding, mold flow analysis, and the promise of using the 3D printing process for mold fabrication. In the second part, they demonstrate the injection molding process using 3D printed polymer molds and its suitability for low-run productions. 3D printed molds using stereolithography and fused filament fabrication have been injected with poly(lactic acid), and the quality of the injected parts was assessed in terms of dimensional accuracy and the damage mechanisms during fabrication. doi.org/10.1557/mrc.2019.147

Integrating lattice materials science into the traditional processing–structure–properties paradigm

Frank Zok, University of California, Santa Barbara, USA

Periodic lattice materials have been studied extensively in numerous science and engineering fields. Despite the vast knowledge that has emerged, the activities have been stove-piped within individual research communities, often in isolation from those in related fields. To bring this work into a holistic framework, the present article considers the elements needed to integrate the study of lattice materials into the processing–structure–properties paradigm that underpins materials science as an academic discipline. The emphasis is on concepts of structure involving topology, morphology, and defects of lattice materials, with illustrations of structure–property relations in the context of lattice strength. doi.org/10.1557/mrc.2019.152

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RESEARCH LETTERS

Preparation of graphene oxide-reinforced calcium phosphate/calcium sulfate/methylcellulose-based injectable bone substitutes

Öznur Demir Oğuz, **Duygu Ege**, Boğaziçi University, Turkey

In this study, an injectable bone substitute (IBS) was produced by mixing a liquid and powder phase. The liquid phase consisted of 8 wt% methylcellulose (MC), 2.5% gelatin, and different amounts of graphene oxide (GO). The powder phase was composed of tetracalcium phosphate (TTCP), dicalcium phosphate dihydrate (DCPD), and calcium sulfate dihydrate (CSD). The results showed that 1 and 1.5 wt% GO added IBS samples showed higher stability, injectability, rheological properties, and biocompatibility than the other GO added IBS samples. GO addition significantly decreased the setting time, but it did not significantly affect the compressive strength of the samples.
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Piezoelectric bioMEMS cantilever for measurement of muscle contraction and for actuation of mechanosensitive cells

Elizabeth A. Coln, **Alisha Colon**, University of Central Florida, USA; **Christopher J. Long**, **Narasimhan Narasimhan Sriram**, Hesperos, Inc., USA; **Mandy Esch**, **Jean-Matthieu Prot**, Cornell University, USA; **Daniel H. Elbrecht**, University of Central Florida, and Cornell University, USA; **Ying Wang**, Cornell University, USA; **Max Jackson**, Hesperos, Inc., USA; **Michael L. Shuler**, Hesperos, Inc., and Cornell University, USA; **James J. Hickman**, University of Central Florida, and Hesperos, Inc., USA

A piezoelectric biomedical microelectromechanical system (bioMEMS) cantilever device was designed and fabricated to act as either a sensing element for muscle tissue contraction or as an actuator to apply mechanical force to cells. The sensing ability of the piezoelectric cantilevers was shown by monitoring the electrical signal generated from the piezoelectric aluminum nitride in response to the contraction of iPSC-derived cardiomyocytes cultured on the piezoelectric cantilevers. Actuation was demonstrated by applying electrical pulses to the piezoelectric cantilever and observing bending via an optical detection method. This piezoelectric cantilever device was designed to be incorporated into body-on-a-chip systems.
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Enhancing ionic conductivity with fluorination in organosilyl solvents for lithium-ion battery electrolytes

Leslie J. Lyons, Tom Derrah, **Steven Sharpe**, **Seiyoung Yoon**, **Scott Beecher**, Grinnell College, USA; **Monica Usrey**, **Adrián Peña-Hueso**, **Tobias Johnson**, **Robert West**, Silatronix, Inc., USA

Increasing fluorination of organosilyl nitrile solvents improves ionic conductivities of lithium salt electrolytes, resulting from higher values of salt dissociation. Ionic conductivities at 298 K range from 1.5 to 3.2 mS/cm for $LiPF_6$ salt concentrations at 0.6 or 0.7 M. The authors also report on solvent blend electrolytes where the fluoroorganosilyl (FOS) nitrile solvent is mixed with ethylene carbonate and diethyl carbonate. Ionic conductivities of the FOS solvent/carbonate blend electrolytes increase achieving ionic conductivities at 298 K of 5.5–6.3 mS/cm and salt dissociation values ranging from 0.42 to 0.45. Salt dissociation generally decreases with increasing temperature.
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Noninvasive oral cancer detection from saliva using ZnO–rGO nanocomposite-based bioelectrode

Shilpi Verma, **Surinder P. Singh**, Academy of Scientific and Innovative Research, and CSIR-National Physical Laboratory, India

Multifunctional materials with excellent biocompatibility and electron-transport properties are critical for the pursuit of point-of-care biosensing devices. The authors report the synthesis of zinc oxide–reduced graphene oxide (ZnO–rGO) nanocomposite for the fabrication of an electrochemical immunosensing test bed for noninvasive on-site detection of an oral cancer biomarker (interleukin-8, IL8). The immunosensor showed successful detection of IL8 at low concentration ranges, that is, 100 fg/mL–5 ng/mL with a sensitivity of 12.46 ± 0.82 μA mL/ng and a detection limit of 51.53 ± 0.43 pg/mL. These results have been validated through *in vitro* investigations using real saliva samples spiked with IL8.
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Printable ionizing radiation sensors fabricated from nanoparticulate blends of organic scintillators and polymer semiconductors

Darcie Anderson, **Sophie Cottam**, **Heidianne Heim**, **Huiming Zhang**, **Natalie P. Holmes**, **Matthew J. Griffith**, The University of Newcastle, Australia

This work established the feasibility of flexible solution-processed radiation sensors prepared from an organic scintillator (1-phenyl-3-mesityl-2-pyrazoline) and a biocompatible semiconducting polymer (violanthrone-79). Absorbance, steady-state, and time-resolved photoluminescence measurements demonstrated a high efficiency for the transfer of absorbed energy from the scintillator to the semiconductor. Blended nanoparticles containing both materials were fabricated in order to reduce the intermolecular distance between molecules, creating a highly efficient energy-transfer pathway. Radiation-sensing devices were then constructed from the materials. These exhibited successful sensitivity for gamma radiation from a ^{137}Cs source that was not present for the control semiconducting polymer alone.
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Tunable neuronal scaffold biomaterials through plasmonic photo-patterning of aerogels

Martina Rodriguez Sala, **Chenhui Peng**, **Omar Skalli**, **Firouzeh Sabri**, University of Memphis, USA

The authors have shown that the neurite extension by neuronal PC12 cells is greatly impacted by aerogel topography. Indeed, the average neurite length of PC12 cells grown on aerogels is greater than that in cells cultured on control substrates. Here, the authors report on the first experimental study focused on the design and development of a plasmonic photo-patterning technique for collagen-coated mesoporous aerogel biomaterials. Herein, the authors have produced specific patterns on silica aerogels by performing precise plasmonic photo-patterning on liquid-crystal-coated aerogels. They report the methodology employed to create a collagen–liquid-crystal gel mixture imprinted with precise plasmonic photo-patterns. PC12 cells plated on these patterns did attach and survive and followed the spatial cues of the pattern to align themselves in a similar pattern.
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