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Form and Function of Disorder

Dedicated to Professor David A. Drabold on the occasion of his 60th birthday

Since Anderson's seminal paper "Absence of diffusion in certain random lattices" [*Phys. Rev.* 1958, *109*, 1492] and its subsequent generalization by Mott to disordered electronic systems more than half a century ago, an extensive progress was made in the study of disordered condensed matter physics in the past decades. Mott's realization that electrons in disordered solids can be described by localized wave functions and the existence of mobility edges—the energy boundaries separating the extended and localized states—in the density of electronic states lead to the conclusion that a disordered solid can undergo a metal-insulator transition at zero temperature in the presence of sufficient disorder. The work of Mott and others opened up a new vista in condensed matter physics that resulted in remarkable achievements in the study of disorder and electronic correlations in solids in the decades to follow. The absence of translational symmetry in disordered solids implies that the cornerstone of the old solid state physics—the Bloch theorem—is no longer valid and so is the very concept of energy bands, on which the entire edifice of the $\boldsymbol{k}$-space-based old theory is built upon. However, the vacuum was immediately filled by local approaches to electronic structure of solids in real space, where great emphasis was placed on bond order and density matrices. Of particular importance are the local approaches adopted by the French school under the leadership of Friedel, and Heine and others in the United Kingdom. These researchers have shown that the structure and electronic properties of noncrystalline solids can be effectively addressed from a chemist's bonding point of view by using advanced scattering theory and Green's functions. A description of electronic properties of disordered solids then naturally emerges from the local density of states and density matrices instead of energy bands. The importance of the density of states in studying disordered solids is perhaps most elegantly expressed by a theorem, due to Cyrot-Lackmann, that connects the moments of the local density of states to the topology of the local atomic environment of a network.

Viewing the subject in the light of its development over a period of the past five decades, it is evident that the field of disordered materials continues to present significant challenges and problems of outstanding interest to date. While the generic behavior of many disordered systems is now more or less understood, our knowledge and understanding of the properties of real disordered materials are still evolving and far from being complete. From a theoretical point of view, the main difficulty arises from the lack of knowledge of atomic positions in disordered solids. Diffraction experiments, while provide useful structural information through atomic pair-correlation functions, alone cannot determine the three-dimensional structure of

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disordered solids via inversion of pair-correlation data. In view of this, the great majority of current theoretical methods for structural inference of disordered solids are limited to Monte Carlo and molecular-dynamics simulations, using a variety of total-energy functionals from classical and semi-classical to quantum-mechanical approaches. The last approach mostly relies on the density-functional theory (DFT), developed by Kohn and Sham in the sixties. While these approaches have been highly successful in determining structures and properties of many disordered solids, such as structural glasses, they are nonetheless limited to either small system sizes (via DFT calculations) or relatively simple amorphous/glassy solids for which accurate classical or semi-classical force-fields are available. The computational complexity associated with DFT calculations for large disordered systems continues to present a major obstacle in studying complex multi-component glasses of technological importance. Metallic glasses are classic examples in this category, the properties of which are often characterized by medium-range ordering on the nanometer length scale. Likewise, the interplay between magnetism and disorder remains largely an uncharted territory. While sophisticated theories of magnetism (for disordered materials) are already in place, a unified approach that simultaneously takes into account structural disorder and magnetic interactions between atoms is still missing.

In recent years, the emergence of a new breed of computational methods, which rely on experimental data and relevant structural information, brings fresh impetus to address the

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problem of materials modeling from a data-centric point of view. These data-driven methods either construct a machine-learning (ML) potential, using a set of training data from a small number of high-quality DFT simulations and experiments, or generate realistic models of disordered solids by directly incorporating a set of experimental data and (approximate) total-energy functionals in an augmented solution space. Although it remains to be seen to what extent ML approaches can address some of the most difficult problems in materials modeling, involving multi-component glasses in a non-stoichiometric environment with associated length- and time-scale issues, there is a cautious optimism in the air that ML approaches can bring a paradigm shift in computational materials discovery. While we wait for the future to deliver a definitive answer, it is undoubtedly an exciting time for studying disordered materials when new data-driven methods and experimental results are reported regularly.

The current issue "Form and Function of Disorder" originates from our desire to honor and celebrate the sixtieth birthday of Professor David A. Drabold and his contributions in this field. Although we had to cancel the accompanying conference (May 30–31, 2020 in Athens, Ohio, USA), due to the outbreak of Covid19 pandemic in 2020, we are delighted that the special issue has finally come to fruition irrespective of the pandemic-related difficulties that we have experienced recently. The issue consists of twenty-two (22) articles of which fourteen (14) are directly related to the study of disordered systems/materials. The topics covered are diverse in nature and they range from applications of classical, quantum-mechanical, and ML approaches to glasses of technological interest, as well as generic understanding of disordered systems from geometric and topological points of view.

Following our discussion on emerging methods and their applications, and noting the limited availability of space, we briefly mention here a small number of articles that are thematically related to the title of the issue. The article by Konstantinou et al. (pssb.202000416) illustrates the use of machine-learning potentials with DFT accuracy in studying a phase-change material, Sb_2Te_3, whereas the application of a data-assisted FEAR approach is presented by Thapa et al. (pssb.202000415) to study an important metallic glassy system, Cu46–Zr46–Al8. The transition from glasses to crystalline structures is discussed by Sun et al. (pssb.202000427), where the authors examine the evolution of the interface between glassy and crystalline structures in lithium disilicate systems. The work by Dahal et al. (pssb.202000447) explores the origin of the fast sharp diffraction (FSDP) peak in amorphous silicon and provides some new insights on the relationship between the position of the FSDP in the wavevector space and a radial length scale in real space. Subedi et al. (pssb.202000438) discuss a fascinating approach to employ the Kubo-Greenwood formula for studying conductivity in amorphous solids that leads to identification of conductivity paths/regions in real space via construction of a conducting matrix. The article by Biswas (pssb.202000610) addresses the structure of energy landscapes of some highly degenerate model spin-glass systems. The author presents a new classification scheme by providing a two-dimensional description of high-dimensional potential-energy surfaces, showing the energy minima and barriers that separate them. The nature of atomic vibrations in models of vitreous silica has been studied by Shcheblanov et al. (pssb.202000422) with an emphasis on the low- frequency vibrational modes. The authors show that the modes are quasi-localized in nature and resulted from a mixing of non-localized and localized vibrational states. The latter have been found to exhibit both exponential and power-law decays. The article by Sadjadi et al. (pssb.202000555), on isostatic material frameworks, provides a brilliant discussion on how topological and geometric constraints in random networks can play a decisive role in understanding some generic properties of real disordered materials. The remaining articles are equally fascinating and enjoyable to read.

We thank the authors for delivering a high standard of scientific content in their articles for this special issue. Finally, we are grateful to the editorial team of *physica status solidi (b)*, and in particular Dr. Sabine Bahrs, who worked alongside us for the past year to make this issue finally appear in print.

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Gang Chen received his Ph.D. in Materials Science and Engineering at Lehigh University (Bethlehem, PA, USA) in 2004. He is currently an Associate Professor in the Department of Physics and Astronomy at Ohio University (USA). His research is focused on fundamental understanding of the structure–property relations in amorphous electronic materials.

Serge Nakhmanson's research interests involve modeling of functional materials properties using quantum-mechanical and finite-element based computational tools. He is one of the original creators and a developer of the 'Ferret' code for simulating ferroic functionalities at mesoscale. Specific areas of interest include novel multifunctional materials and predicting their behavior; influence of shape, size and orientation on the material properties, as well as occasional excursions into "soft" ferroelectrics, such as polymers, oligomers and molecular crystals.

Jianjun (JJ) Dong is a Professor of Physics at Auburn University (Auburn, AL, USA). He received his Ph.D. degree from Ohio University in 1998, under the supervision of Prof. David Drabold. His research focuses on theories and simulations of real materials. A current research thrust is to develop new theories and computational methodologies to understand heat transfer properties of materials, such as materials at extreme low or high temperatures, very anharmonic crystals, disordered/glassy solids, and material interfaces.