A Perspective on Intelligent Design of Engineered Materials and Structures by Interface Mechanics

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Abstract: Engineering design of materials and structures has evolved radically from earliest employment of single phase materials with a focus on optimization of geometric shapes to recent multiphase materials with tactful integration and assembly in both geometric shapes and material domains. In these recent design concepts and strategies, the interfaces are crucial and leveraged to achieve properties and functionalities surpassing those of individual material/phase components and/or their simple superpositions. This perspective focuses on the underpinned interface mechanics view in which insights are essential to understand fundamentals of integration, tailoring and assembly of multiphase materials with diverse geometric layouts. The view also provides insights to enable creations of intelligent new design concepts and approaches of materials and structures capable of being readily manufactured with current technologies. Selected examples of engineered materials and structures enabled by either solid-solid or solid-liquid interactions are provided to highlight the driving role of interface mechanics in designs and to outlook the associated future opportunities and challenges.

Key words: Materials and structures by design; Interface mechanics; Solid-solid interaction; Solid-liquid interaction; Perspective

Introduction

Materials and structures by engineering design have proven to be a powerful strategy to accelerate the discovery of new materials and to achieve the overwhelming material properties and functionalities including high flexibility, large stretchability, super-high toughness and strength, self-healing, ultralight weight, and fast response, to name a few. Especially over the recent years, it has largely been motivated by engineering applications in energy and environmental

sustainability, healthcare, robotics, as well as security, and also has strongly been supported by innovative advances in manufacturing techniques. Meanwhile, ever-growing demands to properties and functionalities of materials and structures have rapidly shifted from one single functionality on individual materials and structures such as high strength, fracture toughness, negative Poisson's ratio, superhigh thermal conductivity, to multifunctionality such as high-strength and lightweight materials, mechanically stretchable and thermally stable electronics, electrically conductive and mechanically tough polymers, environmentally responsive and mechanically self-protective systems. These shifts to multifunctional properties usually cannot be achieved by employing one single material component, and relies strongly on intensive involvements and seamless integrations of multiple phase materials by design. The exploratory design concepts, approaches and strategies for multi-materials are considered to shape the future intelligent design of multifunctional materials and structures.

In the efforts of these designs, the interfaces in integration and assembly boundaries between either different material components or geometric shapes of assembly units that are closely associated with deformation mismatch, interfacial wetting, and molecular diffusion and intrusion will be of critical importance to achieve on-demand properties and functionalities of engineered materials and structures. Compartmentalizing and leveraging these elementary interface features and their underlying interface mechanics principles could result in new, intelligent design principles for functional materials, structures and systems. Here, we will focus on interface mechanics-enabled approaches in design of engineered materials and structures by highlighting unique characteristics in interface integration and interactions between both solid-solid and solid-liquid materials.

Results

Engineering design by solid-solid interfaces

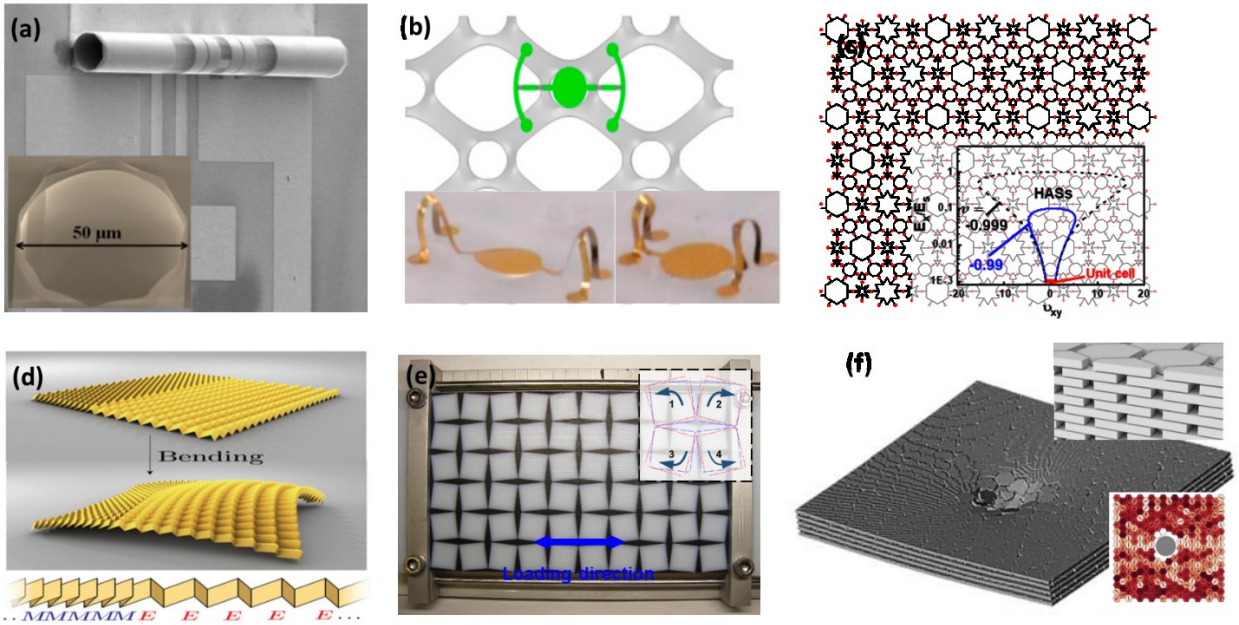

Figure 1: Functional materials and structures enabled by tailoring solid-solid materials. (a) Self-rolled-up composite membrane led by interface mismatch of well-adhered layer materials after releasing its pre-deposited planar form from substrate[1]. **(b)** Popped-up mesostructure with diverse spatial morphologies by controlling its bonding locations on substrate or/and the releasing paths of the pre-strain applied to substrate[2]. **(c)** Heterogeneously architected planar structures exhibiting a super-large range of Young's modulus and Poisson's ration by positioning their unit cells or/and controlling their interface connections[3]. **(d)** Hybrid origami with programmable deformation models and mechanical properties by tailoring unit cells in Miura (M) and in eggbox (E) mode[4]. **(e)** Mechanical auxetic structure enabled by hard particle rotation in soft matrix[5]. **(f)** Tough laminated glass enabled by the sliding mechanism of tablets across interfaces[6].

Figure 1a shows a self-rolled-up membrane for applications in designing three-dimensional radio-frequency transformers[1]. The membrane is made of several different, well-arranged material layers. The self-rolling results from material mismatch of layer components once the pre-deposited planar membrane is released from substrate. The difference of mechanical stiffness between layers determines the diameter of the rolled-up structures. The number and orientation of turns can be controlled through in-plane patterns or layouts in each layer. The mismatch-induced overall deformation on structures is controlled by selective design of interface boundaries. Similarly, through a skillful selection of materials and geometric patterns, structures with various spatial morphologies have been designed by controlled wrinkling, buckling or folding[7-9]. The interface mismatch can also be triggered and regulated by external stimuli, including thermal loading, mechanical loading, electrical field, magnetic field, and pH value.

Figure 1b presents a three-dimensional popped-up mesostructure by releasing the pre-strains applied to the substrate[2]. The spatial morphologies of mesostructures can be well designed by programming the loading and releasing direction or/and the sequential order of the pre-strain applied to substrates. The careful design to pop-up locations and interface adhesion strength between film membranes and substrates can extensively enrich the popping-up paths and deformation modes. The variety of these paths and models will further promote the design parameter space of popping up three-dimensional structures with desirable properties and functions for various applications[10-12]. Besides, with the employment of responsive materials of either film membranes or substrates, the popping process, popped structures or structural shapes by design could be dynamically transformable, adaptive to external environments[13-15].

Compared with the out-of-plane mechanical deformation by material mismatches at interface, it has also been utilized to design materials and structures with excellent mechanical properties capable of being programmed through simple arrangements of unit cell components. **Figure 1c** illustrates an example of designing heterogeneously architected structures (HASs) by harnessing deformation mismatch of assembled lattice unit cells[3]. The HASs exhibit an extremely broad range of mechanical properties. For example, both Young's modulus and Poisson's ratio of designed HASs can vary from nearly zero to three orders of magnitude higher than individual cell components. This spanning range can be further enlarged by on-demand design to interface connections between basic lattice cells. Similar principles have been applied to design three-dimensional architected lattice structures for constructing lightweight and strong materials, and high-efficient energy dissipation performance [16-18]. As another example, **Figure 1d** presents a hybrid origami assembled by a half unit cells in Miura (*M*) mode and the other half in eggbox (*E*) mode[4], where the *M* and *E* mode unit cells have contrasting Poisson's ratios. The integrated interface between the unit cells coordinates and determines the overall deformation modes and mechanical properties of the hybrid origami. As such, a topological deformation mode locking and continuously tunable switching of Poisson's ratio can be well designed by programming assembly interfaces associated with arrangements of *M* and *E* modes. Similarly, tailoring the unit cells with contrasting mechanical properties has helped design mechanically tunable thermal structures, where the stress distribution near the assembly interface offers a regulation means by mechanical loading[19].

Biological materials in nature offer a powerful inspiration source for material design. However, pinpoint duplication of biological structures to design materials and structures in engineering is fairly limited. The key reason is a lack of complete and rigorous understanding of properties of biological materials across a large span of multiscale structures with numerous both geometric and material interfaces[20-23]. Selective bioinspiration design that focuses on key features of biological materials with limited interfaces provides an alternative approach. **Figure 1e** shows a 3D printed soft-hard material integrated mechanical metamaterial, where an auxetic design is achieved by the rotation of hard particles in soft matrix[5]. This auxetic design is inspired by biological material nacre[24], but only leverages its soft-hard materials integrated features. This particle rotation-enabled design mechanism is closely dependent on soft-hard integrated interfaces and has also been utilized to design mechanically tunable phonon crystals[25] and metasurfaces[26]. When responsive particles or active soft matrix to external fields are employed in design, the particle rotation will help improve the actuation efficiency of materials and structures[27]. Further, **Figure 1f** illustrates a bioinspired design of laminated transparent glass duplicating the three-dimensional brick-and-mortar arrangement of nacre from mollusk shells[6]. Different from the rotation mechanism in Figure 1e, upon an impact loading, sliding along interfaces between tablets facilitates the nonlinear deformation and significantly improves toughness of the engineered glass. This interfacial sliding mechanism can be controlled by either tuning geometry of tablets or applying a pre-strain, and has been used to design architectured structures with improved strength and deformation stability [28, 29].

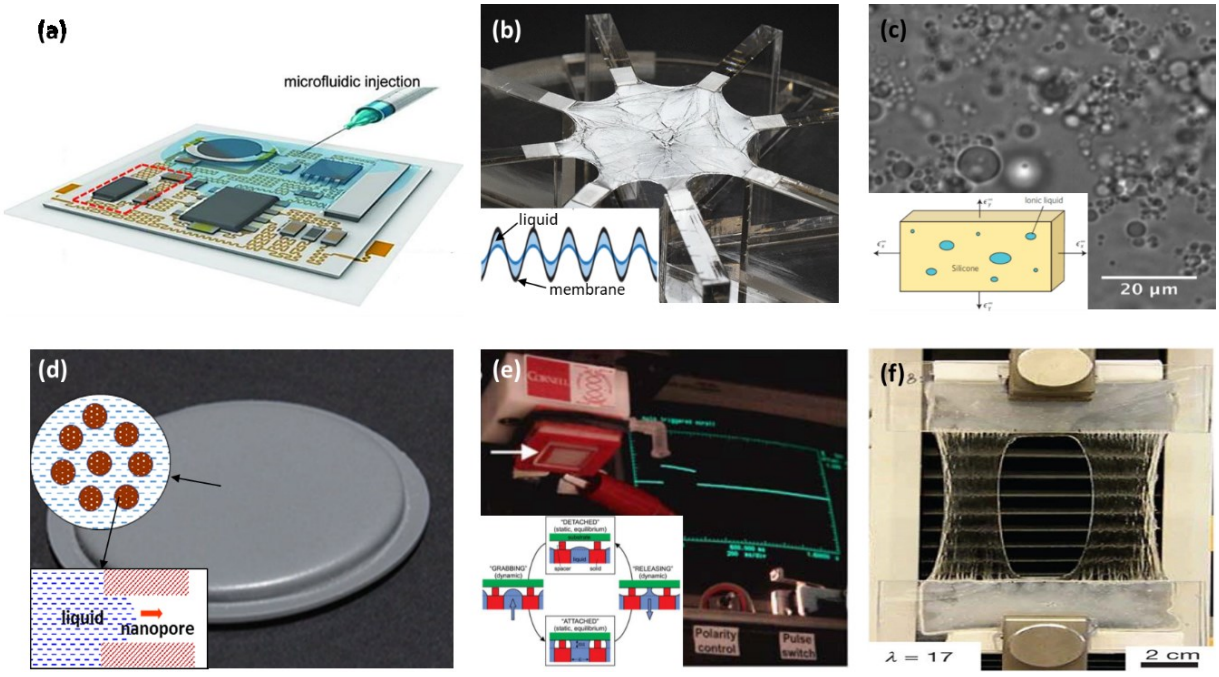

Figure 2: Functional materials and structures enabled by tailoring solid-liquid materials. (a) Soft, stretchable electronic system that lays solid device components and their interconnection wires in a liquid substrate[30]. **(b)** Ultrastretchable wicked membrane with the fibrous membrane infused by wetting liquid[31]. **(c)** Soft yet stiffened solid enabled by the embedded liquid droplets [32]. **(d)** High-performance energy dissipation/capture system comprised of nanoporous materials suspended in a non-wetting liquid environment, all sealed inside a polymer film [33, 34]. **(e)** Electrical capillarity based, switchable wet adhesion system [35]. **(f)** Highly stretchable and tough hydrogel with the containment of ~90% water[36].

Engineering design by solid-liquid interfaces

Integrating solid-liquid materials, where either liquid is embedded into solid materials or solid is suspended in liquid matrixes, has provided an alternative design approach to achieve excellent, novel material properties and functionalities, and the underlying design key is the solid-liquid interface. Especially, the solid-liquid interface under a confined environment provides a unique interface and enables novel solid-liquid integrated materials and structures, beyond the material design by traditional wetting theory.

Figure 2a illustrates a soft wearable electronic system comprised of solid device components and their interconnection wires, all encapsulated on a microfluidic substrate[30]. This solid-liquid interaction leads to the free-floating interconnects that can buckle, twist and deform with nearly no constraint in response to externally imposed deformations of the entire system. The fluidity interface associated with this solid-liquid interaction has also been utilized to design

material and film assembled systems[37, 38]. Leveraging solid-liquid interactions in a constrained space has also led to novel materials and systems. **Figure 2b** shows an ultra-stretchable wicked membrane with fibrous membrane infused by a wetting liquid[31]. The interactions between solid membrane-wetting liquid render local folding, wrinkling and stacking of membrane and formation of venation network with ruffles and furrows, and the rough network buffers the excess membrane and mediate stretching deformation. Depending on the thickness of solid membrane and liquid space, this solid-liquid interaction mechanism could mediate stretchability as high as eight times higher than that of solid membranes only. Similar mechanism is applied to design thin film-liquid materials with tunable compression and bending capabilities[39]. In particular, the interplay between elasticity of solid materials and interfacial interaction-induced capillarity is well harnessed to design extensible liquid wires[40], where solid filaments are buckled and folded within the liquid droplets and are unfolded for extension upon a stretching. The associated capillary forces due to this solid-liquid interaction have provided an unique design principle to achieve engineered materials and structures with a broad range of geometric shapes[41, 42]. Different from this liquid with free fluidity, the discrete liquid phase such as droplet has been embedded into solid materials for functional material design. **Figure 2c** presents a soft solid with spherical liquid inclusions[32]. When the finite concentration of embedded liquid droplets is smaller than the elasocapillary scale, the stiffness of soft solids will be significantly enhanced due to the surface tension of liquid at interface. Further study reveals that the non-spherical shape of liquid inclusion may soften soft solids[43]. In addition to surface tension, when the liquid of embedded droplets changes from water to liquid metals, or to complex fluids, solid-liquid interaction mechanisms such as liquid diffusion across interfaces become important and have been utilized to guide the design of soft-liquid composite materials with various properties and functions[44-46].

By comparison, solid materials can be immersed into liquid phase in functional materials by design. **Figure 2d** shows a liquid foam sealed inside a polymer film[33, 34]. This liquid foam is comprised of nanoporous particles fully suspended in a non-wetting liquid. Due to hydrophobic nature of solid nanoporous materials, the liquid cannot intrude into nanopores unless an external stimulus such as voltage, heat, or pressure is applied to regulate the solid-liquid interfacial energy. Because of ultra-large specific surface area of nanopores (~1000 m^2/g), upon the intrusion and extrusion of liquid into and out of nanopores, this liquid foam provides a very attractive material

and system for high-performance energy conversion and storage[47]. Similar mechanisms of solid-liquid interactions in a confined environment have been employed to design energy harvesting devices[48-50], thermal actuators[51], and field effect transistors[52]. Because of controllable response of solid-liquid interactions to external fields, the cyclic status of liquid in and out of micro/nanochannels has been designed to a smart system[53, 54]. **Figure 2e** shows an example on a capillary based switchable adhesion device system, where the solid-liquid interaction is tuned through an external electrical field[35]. The strong adhesion of device grabs is activated when liquid is actuated out of microchannels to form a large number of small bridges for contact between devices and substrates to be grabbed; breaking the contact will lead to the release of substrate, making the adhesion switchable. Compared with the employment of a clear interface of liquid at solid surfaces, the supply of liquid can blur the solid-liquid interfaces due to swelling or degradation of solids associated with infiltration of liquid into solid materials, in particular, soft materials, and is utilized to design adhesion materials[55-59].

In addition, at the molecular level, the solid-liquid interactions have enabled many designs of soft materials with desirable properties and functionalities such as hydrogels. **Figure 2f** shows a highly stretchable and tough hydrogel with the containment of ~90% water[36]. With the regulation to wettability of polymer molecules, size of polymer networks or employment of responsive groups, the solid-liquid interactions can be substantially changed[60-62], which enables the design of a class of unique hydrogels such as self-healing hydrogels[63], anti-fatigue hydrogels[64], and stimuli-responsive hydrogels[65].

Challenges and opportunities

Although materials and structures by engineering design has a long history, fast-growing demands toward multifunctionalities are calling for new design principles and approaches for innovations that require seamless integrations and assemblies of different material/phase components with subtle geometric optimizations. These examples highlighted above suggest that interface mechanics associated with either solid-solid or solid-liquid integrations provides unprecedented solutions to advance material and structural designs. On the other hand, the re-emerging and prosperous growth of materials and structures by design will bring grand opportunities to interface mechanics that requires intensive and close endeavors from theory,

computation, to experiment. As such, developments of precision theoretical models of interface mechanics must integrate the complexity of interface boundaries both geometrically and physically. Multiple shaped interfaces usually co-exist in engineered materials and structures by solid-solid integrations. The deformation coordination at and the information exchange across interfaces determine properties and functionalities of overall engineered materials and structures, where full descriptions of the associated interface mechanics theories could be established through statistical or topological approaches. More importantly, when the interfaces are down to nanosize, the factors associated with atomic reaction/diffusion, surface energy, thermal transport, and charge transfer must be integrated in the development of multiscale, multiphysics interface mechanics models. For solid-liquid integrated materials and structures by design, it involves the interlocked coupling of fluid dynamics of liquid and mechanical deformation of solids. Therefore, the underpinned solid-liquid interfaces are usually not fixed and keep instable, where solid materials such as soft materials will deform due to liquid fluid-induced forces[66], and subsequently, the deformed solids will change flow fields. Especially, when solid materials such as porous materials are in contact with liquids, the intrusion and extrusion of liquid, or even evaporation of liquid makes interfaces dynamically changeable[67, 68]. It is crucial for interface mechanics models to incorporate solid and fluid mechanics down to the nanoscale. Moreover, phase change for functional liquid or liquid in a nanoconfined environment may happen[69], and additions/improvement of associated this change to interface models will be very necessary. In addition, when active solid or/and responsive liquids to external environments or manipulation means such as heat, voltage, magnetism, force, and pH value are employed in design, energy analysis could offer an alternative and more lucrative way to help develop theoretical themes of interface mechanics.

The advance of material and structural design by interface mechanics also offers exciting opportunities for computations and simulation modeling, as they are capable of revealing interface properties down to the atomistic scale, thereby advancing design refinements and innovations. The continuous efforts to develop modeling tools and force fields at the nanoscale such as atomistic/molecular simulations that can reproduce the inherent quantum nature at interfaces such as the prediction of chemical reactions [70] and phase transformations [71] at interfaces will be of importance to probe intrinsic mechanisms of materials interactions at interfaces. These nanoscale modeling advances will also help provide direct insights to the theoretical development of interface

mechanics with quantum information coupled. At the continuum scale, finite element analysis needs much efforts to implement theoretical models in connection of domains with multiphysics. Image processing algorithms and skills that help construct realistic finite element models from experimental measurements on microstructures and morphologies of interfaces [72] will also be critical to reproduce properties of engineered materials and structures. More importantly, to close the length and time gaps of computations and simulation modeling between nanoscale and macroscale, the development of multiscale modeling that couples atomistic and continuum information with timely data exchange between each other is a challenge. Especially, in the design of solid-liquid integrated materials and structures, where the interfaces between solid and liquid materials are dynamic with the coupling of mechanical deformation of solid and change of fluid field, computational modeling must take into account these dynamic multiphysics factors. More importantly, in search of optimized design, intensive computational efforts along with a mass of data are usually required. The integration with machine learning tools to pursue data-driven computational modeling will speed up the design with on-demand properties and functionalities in an efficient and low-cost manner. For example, in the design of adhesives by solid-liquid interactions, a data-driven, machine learning assisted computational modeling will be highly needed, not only to minimize the region of atomistic calculations, but also to predict the atomic data information effectively from a database when either solid or liquid changes.

Meanwhile, experimental characterizations and measurements that focus on probing interface characteristics and properties need to be designed. The clean experimental results will not only provide direct validations to theoretical and computational models, but will also offer calibration parameters for modeling enhancements, which both are critical to yield on-demand designs of materials and structures. The novel experimental tools and approaches such as digital image/volume correlation[73-77], nanoprobes[78, 79], in situ holders[80], and tomography[81, 82] serve as the foundation for understanding interfaces of solid-solid interactions at their corresponding scales, yet currently have limitations to uncover features and properties at solid-liquid interfaces. Especially, probing solid-liquid interfaces in response to external fields at the nanoscale is challenging the existing state-of-the-art experiments. For example, environmental transmission/scanning electron microscopes are powerful to elucidate dynamics and deformation of solids in liquid, yet are usually applied in a closed environmental chamber that neither allows

escape of liquid nor responds to external stimuli[83]. In addition, the requirements for continuous and dynamic tracking of either solid-solid or solid-liquid interfaces in both time and spatial spaces frequently lead to massive amount of experimental data. The intensive use of imaging systems has further drastically changed routine post-data analysis in experiments[84]. With such big data sets, similar to computations and simulation modeling, an immediate integration of experimental data analysis with emerging advanced data science approaches such as machine learning will benefit both fast extractions of sought information and eliminations as thoroughly as possible of operational or/and environmental influences such as noises. This integration with highly efficient algorithms, as a return, will help improve experimental designs and measurements.

The engineering design of materials and structures needs synchronous efforts among theory, computation, and experiment. The pursuit of this synergy will help refine each other for improvements in a closed-loop and timely manner, toward the precision design at interfaces in connection of multiple materials. For example, computational and simulation modeling can be established that could reflect the essential design concept of materials and structures through interfacial integrations. Systematic computations are carried out to elucidate the effect of key material and design parameters and their couplings on achievements of desirable properties and functionalities. Upon this elucidation, the completion of experiments will prove the conceptual design of engineered materials and structures and the underlying working mechanism. At the same time, the critical parameters obtained from experiments will be passed into computations and simulations to improve modeling effort. The improvement of modeling work will in turn guide both optimization of material design and experimental settings. Similarly, the synergy between experiment and theory will guide the establishment and refinement of theoretical models including the models to both individual domain of materials and their interfaces. The simulations at the nanoscale will provide the development of theory with mechanism insights and physical parameters that cannot be obtained from experiments. The establishment of theory will serve as the foundation for realizing large-scale computations that generate reliable results for comparison with experiments at the macroscale. In addition, similar to the multiscale modeling, the development of theoretical models with atomistic information inputs will help bridge the results between atomistic simulations at the nanoscale and experimental measurements at the macroscale,

which improve and optimize the engineering design of materials and structures with interfaces across multiple scales.

Concluding remarks

In summary, the fast thriving of multifunctional devices and systems requires tremendous efforts on materials and structures by engineering design that are capable of being readily manufactured by realistic processing and manufacturing strategies, where interface mechanics can play a leading, central role, as evidenced by numerous achievements over the past few years. Especially, the material and structural design enabled by solid-liquid interactions is re-emerging with unprecedented creations of various active solids and complex liquids, where interface mechanics integrates naturally solid and fluid mechanics together. At the same time, innovations of design principles and approaches are stimulating new developments to the study of interface mechanics that brings closer endeavors of multidiscipline including materials, chemistry, physics, manufacturing, and data science.

Looking forward, the prosperity of materials and structures by engineering design will continue without doubt over the next decades. It is also envisioned that its development will be highly catalyzed by leveraging the unique, driving role of the underlying interface mechanics. Some of associated opportunities and challenges with this development include: multiphysics models addressing dynamic exchange of information and deformation across interfaces, especially solid-liquid interfaces in both time and length scales and their response to external environments and stimuli, and modeling and analysis with a close embrace to advanced data science tools addressing time and cost-efficiency in experimental designs and computational setups and the resultant massive data processing. Simultaneously, it is important that innovative design approaches must take into account capabilities and resolutions of manufacturing technologies to interface integrations and assemblies of materials, with the overachieving goal of translating designed materials and structures into practical applications. The continuous work on these aspects will not only improve existing design approaches and concepts, but will also help create new ones toward the development of future intelligent and autonomous design of manufacturable engineered materials and structures. Certainly, these efforts in turn will further advance the study of interface mechanics.

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