2020 International Workshop on "Soft Matter and Biophysics Theories"

Tuesday 15 September 2020 - Thursday 17 December 2020

Institute of Theoretical Physics, Chinese Academy of Sciences

Programme

Title: Onsager principle in polymer dynamics

Speaker: Professor Masao Doi
Affiliation:Center of Soft Matter Physics and its Applications, Beihang University, China
Online: Zoom ID: 518 052 9336, [https://zoom.us/j/5180529336][1]

Abstract: Onsager principle is a variational principle proposed by Lars Onsager in 1931 in his celebrated paper on the reciprocal relation in non-equilibrium thermodynamics. The principle is important in the physics of polymer and soft matter. Almost all kinetic equations which have been used to describe the dynamics of polymer and soft matter systems are derived from this principle. Onsager principle is also useful in solving these equations. Since it is a principle of minimization, it can be used to get approximate solutions of the equations. Here I review the principle from such application point of view. I take examples from capillary hydrodynamics, gel dynamics and flow of viscoelastic fluids.

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[1]: https://zoom.us/j/5180529336

Title: Controlling phase separation in biological cells

Speaker: Dr. David Zwicker
Affiliation:Max Planck Institute for Dynamics and Self-Organization, Germany
Online: Zoom ID:518 052 9336, [https://zoom.us/j/5180529336][1]

Abstract: Phase separation has emerged as an important concept for the spatial organization inside cells. While phase separation explains how droplets form, the traditional, passive descriptions cannot explain how cells control these droplets. To unveil part of this mystery, I will present two different mechanisms used by cells in this talk. I will start by considering chemical reactions that influence the physical properties of droplet components. Driven by the non-equilibrium nature of biological cells, such reactions can stabilize multiple droplets and control their size. I will then focus on the elastic properties surrounding droplets, e.g., provided by the cytoskeleton. I will show that stiffness gradients, which are present in heterogeneous environments like cells, can influence the positioning of droplets and thus determine their overall arrangement. These two examples demonstrate that heterogeneous, living cells can regulate the size, number, and position of their droplets. Moreover, droplets could be controlled in the lab using similar mechanisms.

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[1]: https://zoom.us/j/5180529336

Title: Mechanosensing in cells, or ‘why exercise builds muscles?’

Speaker: Professor Eugene M. Terentjev
Affiliation: Cavendish Laboratory, University of Cambridge, United Kingdom
Online: Zoom ID:518 052 9336, [https://zoom.us/j/5180529336][1]

Abstract: 1. The problem of globular polymer unfolding under applied force is a widely-studied fundamental topic in biological and chemical physics, with important applications in cell biology. Much of the existing literature focuses on the case where force is applied while fixing the opposite end of the polymer chain in space. However, in a realistic biological environment, forces will be applied against viscoelastic references, and the deformation of the folded polymer chain will be combined with the deformation of viscoelastic substrate. This affects unfolding rates, which in turn determines the response of mechanosensors that are based on such unfolding proteins.
2. Sensors are the first element of the pathways that control the response of cells to their environment. Protein complexes that produce or enable a chemical signal in response to a mechanical stimulus are called ‘‘mechanosensors’’. We developed a theoretical model describing the physical mechanism of a reversible single-molecule mechanosensor based on a kinase domain, which initiates the chemical signal in its active phosphorylated conformation, but can spontaneously return to its closed folded conformation when no force is applied. The results compare well with the phenotype observations of cells on different substrates.
3. Skeletal muscles sense internally generated and externally applied forces, and respond to these in a coordinated hierarchical manner at different time scales: we know that exercise builds muscles and long inactivity degrades them. The center of the basic unit of the muscle, the sarcomeric M-band, is perfectly placed to carry out the mechanosensing of different types of load, to which the muscle is subjected. We identify the kinase domain of titin - the giant elastic molecular ruler of the sarcomere - as a candidate for mechanical signalling, and develop the quantitative mathematical model that describes the kinetics of the response, and gives predictions for different regimes of exercise and rehabilitation.

[1]: https://zoom.us/j/5180529336

Title: Single Chain in Mean-field Theory in Semiflexible Polymer Systems

Speaker: Professor Dadong Yan
Affiliation: Beijing Normal University, China
Onsite conference room: 6620, Institute of Theoretical Physics, Chinese Academy of Sciences
Online: Zoom ID:518 052 9336, [https://zoom.us/j/5180529336][1]

Abstract: Single chain in mean-field theory (SCMFT) incorporates the Monte Carlo simulation and the mean-field theory. Instead of solving the modified diffusion equation (MDE), as we do in self-consistent field theory, we can alternatively calculate the path integral in the partition function by the explicit conformation obtained by the Monte Carlo simulation. In this way, we can avoid to solve the high dimensional MDE. The SCMFT has advantage for the semiflexible polymer systems since the semiflexible chain has less conformations, and the calculation will be reduced greatly. In this talk, I will introduce the SCMFT and them show two applications of the SCMFT. One is the compression induced phase transition of nematic polymer brush, while another is the local-exchanged model of polymer crystallization based on worm-like chain model.

[1]: https://zoom.us/j/5180529336

Title: Multicompartment aggregates from self-assembly of miktoarm star quaterpolymers in a dilute solution: A simulation study

Speaker: Professor Baohui Li
Affiliation: Nankai University, China
Online: Zoom ID:518 052 9336, [https://zoom.us/j/5180529336][1]

Abstract: The self-assembly of miktoarm star quaterpolymers, composed of one solvophilic arm and three solvophobic arms connected at a common junction point, in dilute solutions has been investigated using a simulated annealing technique. By tuning the strength of incompatibility between the different solvophobic arms (α) or the quaterpolymer composition, unique multicompartment aggregates are predicted and their formation mechanisms are elucidated. When the three solvophobic arms are of equal length, hexagonally shaped laterally patterned nanosheets always form at large α values. At relatively small α values, transitions from vesicles to nanosheets further to micelles are observed with increasing the volume fraction of the solvophilic arm, fP. The vesicles can be of lateral patterns and with 6 protrusions which distributed symmetrically and each corresponds to a packing defect of the three-colored short-cylinders. Micelles can be highly anisotropic and multiple-patched. The morphological sequence obtained with increasing fP has a similar trend to that obtained with decreasing α. When only two of the three solvophobic arms are of equal length, abundant and intriguing aggregates are predicted by tuning the length ratio between different arms, and α. A at intermediate α value, aggregates such as cuboid-shaped and polygonal-shaped vesicles, cuboid-stacked rods, hexagonally packed nanosheets, rods or spheres patterned with stacked toroids, single helices or double helices, anisotropically patched spheres, and anisotropically patched micelles are predicted. When the value of α gets large enough, sheets with large aspect ratio are always observed at both small and large fP, especially, tetragonal-shaped and polygonal-shaped nanosheets are predicted. The formation mechanisms of the aggregates with special shape and morphology are discussed. Our simulation results are compared with available experiments. The self-assembly of miktoarm star quaterpolymers could provide a powerful strategy for fabricating nano-scaled multicompartment aggregates with special shape and internal morphology which may offer tremendous potential in nanotechnology.

[1]: https://zoom.us/j/5180529336

Title: Correlation between structures and properties in aliquid crystal cell and polymeric systems

Speaker: Professor Chen-Xu Wu
Affiliation:College of Physical Science and Technology, Xiamen University, China
Onsite conference room: 6620, Institute of Theoretical Physics, Chinese Academy of Sciences
Online: Zoom ID:518 052 9336, [https://zoom.us/j/5180529336][1]

Abstract: This talk aims to focus on the correlation between structures and properties in liquid crystal cell and polymeric systems. A Freedericksz-like positional transition is found for a nanoparticle suspended in a liquid crystal cell applied by an external electric field. Other phenomena in polymer brush and hard-soft mixture are also discussed extensively, revealing the specific physical features existing in soft matters.

[1]: https://zoom.us/j/5180529336

Title: Fluctuation theory in polymer physics

Speaker: Professor Bing Miao
Affiliation: University of Chinese Academy of Sciences, China
Onsite conference room: 6620, Institute of Theoretical Physics, Chinese Academy of Sciences
Online: Zoom ID:518 052 9336, [https://zoom.us/j/5180529336][1]

Abstract: Fluctuations are important in the understanding of soft matter/polymer physics. In theoretical physics of polymers, fluctuation effects are best discussed through the statistical field theory, within which fluctuations are captured by the connected correlation functions defined in a coarse grained level. In this talk, I will first review how to formulate a polymer problem in terms of the statistical field theory. Then, I will discuss different phase transitions in polymer systems by resorting to the locality property of the field theory model. Finally, I will discuss an interesting phenomenon, i.e., the thermal Casimir effects in the context of polymer models.

[1]: https://zoom.us/j/5180529336

Title: Understanding Soft Matter for Life

Speaker: Professor Wen-Bing Hu
Affiliation: Nanjing University, China
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Online: Zoom ID:518 052 9336, [https://zoom.us/j/5180529336][1]

Abstract: The lecture will start with Gaia hypothesis to explain the reasons why life needs soft matter. Then three fundamental characteristics of soft matter will be discussed, together with their cutting-edge challenges and potential approaches.

[1]: https://zoom.us/j/5180529336

Title: Unexpectedly strong diamagnetism and super strong paramagnetism of aromatic peptides

due to self-assembling and cations

Speaker: Professor Haiping Fang
Affiliation: East China University of Science and Technology, China
Onsite conference room: 6620, Institute of Theoretical Physics, Chinese Academy of Sciences
Online: Zoom ID:518 052 9336, [https://zoom.us/j/5180529336][1]

Abstract: It has been known for centuries that a large passel of animals navigates using the Earth’s magnetic field. There is a considerable amount of work that shows the biomagnetism of organic components does not include enough ferromagnetic components at the molecular level. In this talk, we show that the diamagnetism of an aromatic peptide, the AYFFF, is greatly enhanced by self-assembling, reaching two orders of magnitude higher than the mass susceptibility of pure water. Moreover, the AYFFF self-assemblies in the chloride solution of some divalent cations (Zn2+, Mg2+, and Cu2+) display super strong paramagnetism, which may approach the mass susceptibility of ferromagnetism. We attribute the observed strong diamagnetism and super strong paramagnetism to the existence of the aromatic rings, and the interaction between the aromatic rings and the cations through cation-π interaction.

[1]: https://zoom.us/j/5180529336

Title: Effect of packing frustration on the self-assembly of block copolymers

Speaker: Professor Weihua Li
Affiliation: Fudan University, China
Onsite conference room: 6620, Institute of Theoretical Physics, Chinese Academy of Sciences
Online: Zoom ID:518 052 9336, [https://zoom.us/j/5180529336][1]

Abstract: Packing frustration of polymer chains, originating from a competition between the need to uniformly fill the space and the tendency to minimize the interfacial area, commonly exists in the self-assembly of block copolymers, especially for the formation of nonlamellar ordered structures. We propose to control packing frustration by designing the architectures of block copolymers, and thus to regulate the self-assembly behaviors. The basic idea of controlling packing frustration is to fill the matrix space using different blocks in length. In particular, the packing frustration is largely released when short and long blocks are locally segregated to fill the far and near spaces, respectively. Our results of self-consistent field theory demonstrate that the effect of packing frustration can be applied to tuning the relative stabilities between different ordered phases, and even to stabilizing unusual ordered phases.

[1]: https://zoom.us/j/5180529336

Title: Complex plasma: the plasma state of soft matter

Speaker: Professor Chengran Du
Affiliation: Donghua University, China

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Online: Zoom ID:518 052 9336, [https://zoom.us/j/5180529336][1]

Abstract: Complex plasmas, composed of weakly ionized gas and microparticles, represent the plasma state of soft matter. The particles are usually negatively charged due to the high thermal speed of electrons. Dynamics of individual particles can be easily visualized and measured by the video microscopy. It is an ideal system to study fundamental process in the strong coupling regime on the kinetic level. In the laboratories on earth, the microparticles are usually suspended in the sheath region due to the gravity, forming a particle cluster of single or very few layers with significant inhomogeneity. Performing complex plasma experiments under microgravity conditions can remove this constraint. Without the gravity, it is possible to form a homogeneous 3D particle cluster in the bulk plasma. Many phenomena, which are not accessible on earth, can be then investigated in details.

[1]: https://zoom.us/j/5180529336

Title: The physics and fluid mechanics of dense suspensions

Speaker: Professor Ryohei Seto
Affiliation: Wenzhou Institute, University of Chinese Academy of Sciences
Onsite conference room: 6620, Institute of Theoretical Physics, Chinese Academy of Sciences
Online: Zoom ID:518 052 9336, [https://zoom.us/j/5180529336][1]

Abstract: Dense suspensions, in which rigid particles are dispersed in a viscous liquid at high concentrations, are complex fluids; they flow in peculiar manners. The flow speed is no longer proportional to applied stress or pressure difference. Ultimately, they do not flow in some conditions, called shear jamming. How do they flow? This is a question asking about the material property. Rheology is a study to characterize such properties of complex fluids. Regarding dense suspensions, recent studies succeeded in explaining one of the astonishing non-Newtonian behaviors, shear thickening. However, it is still challenging to predict flows using macroscale continuum simulations. We still do not know how to write a model to relate stress and deformation history for fluid mechanics equations. There may be a fundamental issue of condensed matter physics here. Is it possible to separate material characterization and material behaviors? To have the first step for exploring this question, we extend the previous particle simulation for general flow conditions. We revive the degree of freedom of the solvent flow field, which is fixed in rheology simulations. This new simulation allows us to see the coupling between particle dynamics and the flow of incompressible fluid.

[1]: https://zoom.us/j/5180529336

Title: Computational study of peptide self-assembly, co-assembly and amyloid fibril

disruption

Speaker: Professor Guanghong Wei
Affiliation: Fudan University, China
Online: Zoom ID:518 052 9336, [https://zoom.us/j/5180529336][1]

Abstract: Peptide self-assembly has attracted increasing attention because of its importance in the design of novel biomaterials and its close association with many ageing-related degenerative diseases (such as Alzheimer’s and Parkinson’s diseases) still with no cure yet. Inhibition of the pathological self-assembly (i.e. amyloid fibril formation) of proteins and disruption of preformed protofibrils by natural small molecules are two major promising therapeutic strategies in combating amyloidosis diseases. Unraveling the mechanisms of peptide self-assembly and amyloid fibril inhibition is fundamentally important for the design of bio-inspired nanomaterials and the development of potent drug candidates for the treatment of amyloidosis. Molecular dynamic (MD) simulations play an essential role by allowing generation of sufficiently accurate conformational ensembles which can be used to interpret experimental observations, predict new nanostructures and reveal the molecular interaction mechanisms. Here, I present our recent MD simulation results of peptide self-assembly, co-assembly/aggregation and the molecular mechanisms by which natural small molecules disrupt Aβ protofibrils - the key intermediates of Aβ fibril association and elongation.

[1]: https://zoom.us/j/5180529336

Title: Entropic Strategy in Soft Matter

Speaker: Professor Li-Tang Yan
Affiliation: Department of Chemical Engineering, Tsinghua University, China
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Online: Zoom ID:518 052 9336, [https://zoom.us/j/5180529336][1]

Abstract: Entropy, one of the central concepts of thermodynamics, can be a predominant contribution to structural formation and transition in soft matter. However, due to its statistical nature, fundamental explorations of the entropy underlying various, even counterintuitive, phenomena and establishment of the principles of potential entropic contributions to the structures and activities are scarce and still represent challenging tasks. Here we report our effort on exploring the rules and principles regarding entropy effects in soft matter, including clarifying definitely the entropic ordering and entropic force, defining a new concept of superentropic effect, and proposing the strategy to tune the structural organization by controlling entropic effects though external and internal factors of a system. We finally introduce the applications of such an entropic strategy in some representative soft matter systems, such as enhanced dynamical heterogeneity in semiflexible networks, mechanoresponsive hierarchical assembly of nanoparticle in block copolymers, and the rational design of antibacterial macromolecules.
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1. G. Zhu, Z. Huang, Z. Xu, L. T. Yan. Acc Chem Res 2018, 51, 900.
2. G. Zhu, Z. Xu, L. T. Yan. Nano Lett 2020, 20, 5616.
3. X. Dai, P. Chen, G. Zhu, Z. Xu, X. Zhang, L. T. Yan. J Phys Chem Lett 2019, 10, 7970.
4. P. Chen, Z. Xu, G. Zhu, X. Dai, L. T. Yan. Phys Rev Lett 2020, 124, 198102.

[1]: https://zoom.us/j/5180529336

Title: Bio-inspired mechano-functional gels through multi-phase order-structure engineering

Speaker: Professor Mingjie Liu
Affiliation: Beihang University, China
Onsite conference room: 6620, Institute of Theoretical Physics, Chinese Academy of Sciences
Online: Zoom ID:518 052 9336, [https://zoom.us/j/5180529336][1]

Abstract: Adaptive gel materials can greatly change shape and volume in response to diverse stimuli, and thus have attracted considerable attention due to their promising applications in soft robots, flexible electronics and sensors. In biological soft tissues, the dynamic coexistence of opposing components (for example, hydrophilic and oleophilic molecules, organic and inorganic species) is crucial to provide biological materials with complementary functionalities (for example, elasticity, freezing tolerance and adaptivity). Taking inspiration from nature, we developed a series of high mechanical performance soft active materials, so-called organohydrogels, based on multiphase synergistic strategy. Traditional techniques such as post-polymerization modification, interpenetrating network and controlled micro-phase separation are combined with binary complementary concept to design and fabricate new organohydrogels with diverse topology of heteronetworks. Meanwhile, the synergistic effect of heteronetworks provided the organohydrogels with unprecedented mechanical functions such as freeze-tolerance, programmed high-strain shape memory and shaking insulation. Their applications in anti-biofouling, thin-film fabrication, flexible electronics and actuators are also explored.
References:
1. M. J. Liu et al., Nature, 580, 210 (2020)
2. M. J. Liu et al., Science Advances, 6:eaax 1464 (2020)
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4. Z. G. Zhao et al., Adv. Mater. 29, 33 (2017)
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6. Z. G. Zhao et al., Adv. Mater. 29, 45 (2017)
7. M. J. Liu et al., Nat. Rev. Mater. 2, 7 (2017)
8. M. J. Liu et al., Nature, 517 (2015)

[1]: https://zoom.us/j/5180529336

Title: Physical Principles and Landscape Models of Passive and Active Biopolymers

Speaker: Professor Jin Wang
Affiliation: Stony Brook University, United States.
Onsite conference room: 6620, Institute of Theoretical Physics, Chinese Academy of Sciences
Online: Zoom ID:518 052 9336, [https://zoom.us/j/5180529336][1]

Abstract: In this talk, I will review the recent progresses on the physical principles and landscape modeling the passive biomolecular dynamics such as protein folding, protein recognition and protein conformational dynamics. I will also review the latest developments on the landscape approach and modeling on the active genome structural dynamics for critical cellular functions such as cell cycle, cell differentiation and reprogramming.

[1]: https://zoom.us/j/5180529336

Title: Linker-mediated designed assembly: from colloidal LEGOs to recyclable tires

Speaker: Professor Ran Ni
Affiliation: Nanyang Technological University, Singapore
Online: Zoom ID:518 052 9336, [https://zoom.us/j/5180529336][1]

Abstract: In this talk, I will present our recent work on linker-mediated designed assembly, including the linker-mediated addressable assembly of DNA-coated colloids [Sci. Adv., eaaz6921 (2020)], and the entropy-driven cross-linking in linker-mediated vitrimers [PNAS (2020) arXiv:2007.06807]. I will discuss how we can use linkers as a smart agent to realise the designed precise fabrication on the nano scale as well as to manufacture the new generation of recyclable thermoset polymer materials.
[1]: https://zoom.us/j/5180529336

Title: The Packing of Soft Spheres

Speaker: Professor An-Chang Shi
Affiliation: McMaster University, Canada
Online: Zoom ID:518 052 9336, [https://zoom.us/j/5180529336][1]

Abstract: The packing of spheres is an interesting problem in mathematics and physics with a long history dated back to the work of Kepler and Lord Kelvin. In recent years, intricate periodic and aperiodic spherical packing phases have emerged in a host of soft matter systems including supramolecular assemblies, surfactants and block copolymers, underscoring the universality of emergent order in condensed matter. In particular, the rich phase behavior of block copolymers provides an ideal model system to study the origin and stability of order phases in soft matter. Our recent theoretical study of block copolymer systems revealed that the formation of complex spherical packing phases could be regulated by a number of mechanisms including conformational asymmetry, architecture and variety of the polymeric components. I will summarize recent progresses on this fascinating topic and discuss possible future research directions.

[1]: https://zoom.us/j/5180529336

Title: The growth kinetics of COFs

Speaker: Professor You-Liang Zhu
Affiliation: Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, China.
Online: Zoom ID:518 052 9336, [https://zoom.us/j/5180529336][1]

Abstract: Covalent organic frameworks (COFs) as porous 2D/3D polymers are becoming a central molecular platform to realize the exceptional functions in catalysis, gas separation, energy storage, and etc. However, the surprising difficulty to build the structures with a long-range molecular ordering puzzled researchers. By the aid of molecular dynamics simulations, we studied the growth kinetics of 2D COFs and revealed the mechanisms of defect generation (Nanoscale, 2020, 12, 22107). Further, using Arrhenius two-state model describing reversible reactions, we figured out the conditions in terms of active energy and binding energy for different products including single crystals, polycrystal/crystallites, or amorphous solids (JPCL, 2020, 11, 9952). Finally, we proposed a monomer design strategy to greatly reduce the generation of defects (JPCL, 2020, 11, 179), instead of the correction of defects by reversible reactions.

[1]: https://zoom.us/j/5180529336

Title: Multicomponent glasses and fibers for photonics

Speaker: Professor Shifeng Zhou
Affiliation: South China University of Technology, China
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Online: Zoom ID:518 052 9336, [https://zoom.us/j/5180529336][1]

Abstract: Multicomponent glasses and fibers are considered to be the fundamental building blocks of the next-generation fiber photonics. In this talk, the recent progress in designs, fabrications and applications of selected materials for multicomponent optical glasses and fibers is introduced. In the first part of the talk, the typical microstructures in multicomponent glass system represented by topological features, heterogeneities and locally crystallized domains are discussed. The preliminary results about the relation between the glass microstructure and its optical properties are introduced. In the second part, glasses and glass-ceramics with various optical functions, including photon generation, amplification, modulation and detection are highlighted. Especially, multicomponent glasses and fibers with attractive properties such as tunable, broadband and flat emission are introduced. Their potential applications as gain matrix of broadband fiber amplifier in 5G technology are discussed. In addition, the glasses and fibers with strong radiation blocking ability and intense radiation induced luminescence are introduced. The fiber derived device for radiation detection is highlighted.

[1]: https://zoom.us/j/5180529336

Title: Building the bridge between simulation and experiment of amorphous alloys

Speaker: Professor Pengfei Guan
Affiliation: Beijing Computational Science Research Center, China
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Online: Zoom ID:518 052 9336, [https://zoom.us/j/5180529336][1]

Abstract: Due to the limited spatial and temporal resolution of the current experimental techniques, the study of the heterogeneity in disordered structures, such as amorphous alloys, poses a great challenge. In contrast, computational simulation provides the effective way for understanding the amorphous structure and its response from the atomic level and above. However, due to the complexity rooted in multi-element interactions and the current limitations in computational capabilities, there is still an insurmountable gap between the model systems used in simulations and real amorphous alloys. To address this long-term challenge, one strategy is to integrate the modern computer technology, software and algorithm, which enables exploring and developing more effective computational approaches that can be applied to chemically complex amorphous alloys. In recent years, our group has made progresses in the development of high-efficiency and high-precision computational platform for the simulations of metal-based materials, especially for amorphous materials, through which we successfully performed simulations on a time scale comparable to real experimental time. The outcome of our research cements an algorithmic and theoretical basis to facilitate high-throughput alloy design in near future, including the creation of a database with abundant precise atomic structures and performance data of multi-component amorphous alloys for data-mining.

[1]: https://zoom.us/j/5180529336