Peptide Self Assembly As A Model Of Proteins In The Pre

Peptide Self-assembly on Solid Surfaces
Peptide Bionanomaterials
Tunable Soft Matter Through Peptide Self-assembly
Nanoscale Assembly
Molecular Self-assembly
Peptide Self-assembly
Early-time, Beta-hairpin Peptide Self-assembly and Hydrogelation
Introduction to Peptide Science
Insight Into the Principles of Amphipathic Peptide Self-assembly
Understanding the Fundamental Mechanisms that Drive Amphipathic Peptide Self-assembly
Computational Studies of Sequence-specific Driving Forces in Peptide Self-assembly
Self-Assembly of Peptides, Peptoids, Sugars, & Dendrimers
Self-assembling Cyclic D, L-peptide Nanotubes as Synthetic Transmembrane Channels from Chemical, Biological and Practical Perspectives

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Hierarchical Processes in B-sheet Peptide Self-assembly from the Microscopic to the Mesoscopic Level*Project Supported by the National Natural Science Foundation of China (Grant Nos. 21373270 and 11504431) and the Fundamental Research Funds for Central Universities of China (Grant No. 15CX02025A).
Peptide-Based Materials
Molecular Building Blocks
Artificial Protein and Peptide Nanofibers
Peptide Self-assembly and Engineering
Controlling Long-Range Ordered Self-assembly of Solid-Binding Peptide Monolayers on Atomically Flat Layered Materials
Peptide Based Self-assembled Systems Structures and Applications
Self-Assembling Peptide Systems in Biology, Medicine and Engineering
Self-assembly of Elatin-like Peptides

Self-Assembled Nanomaterials I
Peptide Self-Assembly and Engineering
Molecular Self-Assembly
Self-assembling Biomaterials
Self-assembly of Elastin-like Peptides
Functional and Responsive Materials Exploiting Peptide and Protein Self-assembly
The Assembly and Structure of Self-assembling Peptides
Peptides and Peptide-based Biomaterials and their Biomedical Applications
Self-Assembled Peptide Nanostructures in Materials Chemistry
Self-assembly of Peptides and Peptide Based Hybrids for Therapeutic Applications
Self-Assembled Peptide Nanostructures

KIDD JAZMYN

Peptide Self-assembly on Solid Surfaces
ProQuest
Solid-binding peptides have been used increasingly as molecular building blocks in nanobiotechnology as they can direct the assembly and functionalisation of a diverse range of materials and have the ability to regulate the synthesis of nanoparticles and complex nanostructures. Nanostructured materials such as β-sheet fibril-forming peptides and α-helical coiled coil

systems have displayed many useful properties including stimulus-responsiveness, modularity and multi-functionality, providing potential technological applications in tissue engineering, antimicrobials, drug delivery and nanoscale electronics. The current situation with respect to self-assembling peptides and bioactive matrices for regenerative medicine are reviewed, as well as peptide-target modeling and an examination of future prospects for peptides in these areas. Peptide Bionanomaterials Springer Science & Business Media Understanding the basic mechanisms and dynamics that drive the assembly of molecules into functional structures is critically important in a diverse number of fields, ranging from materials science to drug delivery and biomaterials. In this work, we have focused on examining the self-assembly characteristics, both in solution and at surfaces, of a family of elastin-like peptides (EPs). In addition to directly observing the formation of ordered hexagonally arranged fibrillar EP structures on hydrophobic highly ordered pyrolytic graphite (HOPG), we have studied the dynamics of EP self-assembly process both within physically restricted domains using thermally etched HOPG, and in solution using detergent micelles. We have found that, at surfaces, EP fibril formation occurs via surface stabilization against the hydrophobic surface, while in solution, detergents inhibit EP aggregation at high temperatures and appear to enable the formation of an ordered crystalline

structure at low temperatures. These model studies establish a framework for further investigations of peptide self-assembly and the role of hydrophobic interactions in controlling self-assembly.

Tunable Soft Matter Through Peptide Self-assembly ProQuest

Molecular self-assembly is a creative process in which molecules interact with each other through weak non-covalent interaction in a bottom-up approach and spontaneously self- assemble into a defined arrangement of a larger structure.1-3 This is a fundamental concept of supramolecular chemistry.4 The non-covalent interactions that drive the formation of self- assembled structures are H-bonding, electrostatic interaction, dipole-dipole interaction, n-n stacking, van der Waals force, and hydrophobic effect.5-10 Each of these interactions is weak. However, their collection interactions lead to hierarchical structures.11 From a thermodynamic point of view, these assemblies can be classified into three major categories, in-, out- and dissipative out-of-equilibrium self-assemblies.12-13 In the following sections, I will elucidate the energy landscapes linked with self-assembly processes.

Nanoscale Assembly Humana

The significance of peptide design in the context of self-assembly and its relationship to the nanostructure was studied by designing a series of peptides derived from MAX1. Evolving from these studies is an understanding of the relationship between molecular level

peptide structure and the nanoscale supra-molecular morphology. Based on this, it has been shown that alternate morphologies distinct from those observed with the gel forming peptides, such as non-twisting laminates or tube-like structures can be constructed. Lastly, it is shown that within amphiphilic beta-hairpin peptides, the turn sequence can be used as a design element to control the stiffness of the hydrogel which is an important property from an application point of view. These studies demonstrate that rationally designed peptides are robust building blocks to construct functional materials via molecular self-assembly.

Molecular Self-assembly John Wiley & Sons

Self-assembled peptide nanostructures present a vast potential for materials science. These nanostructures are formed by self-assembly of small molecular weight molecules. Programmed assembly of peptides can be achieved by providing certain inputs at the design level. Noncovalent interactions such as electrostatic interactions, hydrogen bonding, - interactions, solvophobic effects and van der Waals forces can be used as inputs determining fate of a supramolecular ensemble. Supramolecular ensembles can be used as functional templates for the synthesis of hybrid organic-inorganic and purely inorganic nanomaterials. Peptide nanostructures can be utilized in patterning of organic materials as well. For instance, encapsulation of chromophore molecules in peptide

nanostructures presents an interesting approach in controlling photophysical properties of enclosed molecules. Peptide nanostructures have shown great versatility and applicability in materials science. This fact is not surprising, because numerous phenomena taking place in nature actively exploit polypeptides as a handy tool in materials synthesis and its hierarchical organization."

Peptide Self-assembly CRC Press Provides an interdisciplinary introduction to peptide science, covering their properties and synthesis, as well as many contemporary applications Peptides are biomolecules comprised of amino acids which play an important role in modulating many physiological processes in our body. This book presents an interdisciplinary approach and general introduction to peptide science, covering contemporary topics including their applicability in therapeutics, peptide hormones, amyloid structures, self-assembled structures, hydrogels, and peptide conjugates including lipopeptides and polymer-peptide conjugates. In addition, it discusses basic properties and synthesis clearly and concisely. Taking a logical approach to the subject, Introduction to Peptide Science gives readers the fundamental knowledge that is required to understand the cutting-edge material which comes later in the book. It offers readers in-depth chapter coverage of the basic properties of peptides; synthesis; amyloid and peptide aggregate structures; antimicrobial peptides and

cell-penetrating peptides; and peptide therapeutics and peptide hormones. Introduces readers to peptide science, including synthesis and properties Provides unique content covering properties, synthesis, self-assembly, aggregation, and applications Summarizes contemporary topics in an accessible fashion including applications in therapeutics, peptide hormones, amyloid structures, self-assembled structures, hydrogels, and peptide conjugates including lipopeptides Presented at an introductory level for the benefit of students and researchers who are new to the subject Introduction to Peptide Science is an ideal text for undergraduate students of chemistry, biochemistry, and other related biological subjects, and will be a valuable resource for postgraduate students and researchers involved in peptide science and its applications.

Early-time, Beta-hairpin Peptide Self-assembly and Hydrogelation American Chemical Society

Synthesis of Polypeptides by Ring-Opening Polymerization of α-Amino Acid N-Carboxyanhydrides, by Jianjun Cheng and Timothy J. Deming.- Peptide Synthesis and Self-Assembly, by S. Maude, L. R. Tai, R. P. W. Davies, B. Liu, S. A. Harris, P. J. Kocienski and A. Aggeli.- Elastomeric Polypeptides, by Mark B. van Eldijk, Christopher L. McGann, Kristi L. Kiick andJan C. M. van Hest.- Self-Assembled Polypeptide and Polypeptide Hybrid Vesicles: From Synthesis to Application, by Uh-Joo Choe, Victor Z. Sun, James-Kevin Y. Tan and Daniel T.

Kamei.- Peptide-Based and Polypeptide-Based Hydrogels for Drug Delivery and Tissue Engineering, by Aysegul Altunbas and Darrin J. Pochan.-
Introduction to Peptide Science
Woodhead Publishing
Peptide nanotubes are cylindrical, open-ended, ß-sheet supramolecular structures formed from the self-assembly of cyclic peptides that can adopt a flat-ring conformation. In this work, the principles of molecular self-assembly in the lipid bilayer environment are explored through the study of the cyclic peptide nanotubes as synthetic transmembrane channels. Structural evidence for the cyclic peptides as a transmembrane channel is established through an orientational FT-IR analysis of the tubular peptide assembly in the lipid membrane. A biophysical investigation of substituted cyclic peptides using vesicular transport assays, single channel conductance measurements, and attenuated total reflectance FT-IR spectroscopy shows the significant impact of subunit sequence variations on the channel activity and structural organization of the supramolecular assembly in the membrane environment. The potential utility of the cyclic peptides is investigated through a study of their structure and behavior at interfaces, and by the design and synthesis of cyclic peptides with biological activity.
Insight Into the Principles of Amphipathic Peptide Self-assembly John Wiley & Sons
Peptide Self-Assembly and Engineering
State-of-the-art research in peptide self-

assembly, with coverage of fundamental aspects of how peptides self-assemble and an extensive number of applications Peptide Self-Assembly and Engineering: Fundamentals, Structures, and Applications (2V set) covers the latest progresses in the field of peptide self-assembly and engineering, including the fundamental principles of peptide self-assembly, new theory of nucleation and growth, thermodynamics and kinetics, materials design rules, and precisely controlled structures and unique functions. The broad contents from this book enable readers to obtain a systematical and comprehensive knowledge in the field of peptide self-assembly and engineering. Contributed by the leading scientists and edited by a highly qualified academic and an authority in the field, Peptide Self-Assembly and Engineering includes information on: Emerging areas in peptide assembly, such as immune agents, bioelectronics, energy conversion, flexible sensors, biomimetic catalysis, and more Existing applications in biomedical engineering, nanotechnology, and photoelectronics, including tissue engineering, drug delivery, and biosensing devices History of peptide self-assembly for design of functional materials and peptides' unique mechanical, optical, electronic, and biological properties Various solvent conditions, such as pH, ionic strength, and polarity, that can affect the structure and stability of peptide assemblies A very comprehensive reference covering the latest progresses

in the field of peptide self-assembly and engineering, Peptide Self-Assembly and Engineering is an essential resource for all scientists performing research intersecting with the subject, including biochemists, biotechnologists, pharmaceutical chemists, protein chemists, materials scientists, and medicinal chemists.

Understanding the Fundamental Mechanisms that Drive Amphipathic Peptide Self-assembly Humana Nanotechnology has received tremendous interest over the last decade, not only from the scientific community but also from a business perspective and from the general public. Although nanotechnology is still at the largely unexplored frontier of science, it has the potential for extremely exciting technological innovations that will have an enormous impact on areas as diverse as information technology, medicine, energy supply and probably many others. The miniturization of devices and structures will impact the speed of devices and information storage capacity. More importantly, though, nanotechnology should lead to completely new functional devices as nanostructures have fundamentally different physical properties that are governed by quantum effects. When nanometer sized features are fabricated in materials that are currently used in electronic, magnetic, and optical applications, quantum behavior will lead to a set of unprecedented properties. The interactions of nanostructures with biological materials are largely

unexplored. Future work in this direction should yield enabling technologies that allows the study and direct manipulation of biological processes at the (sub) cellular level.

Computational Studies of Sequence-specific Driving Forces in Peptide Self-assembly Springer Science & Business Media

Molecular self-assembly has been exploited by nature for developing the higher functional macromolecular structures of both the genome and proteome. Inspired by nature, there has been a surge of research, in the last two decades, for the molecular engineering of peptide-based self-assembling nanostructures, adopting the bottom-up design approach. This book gives the reader an overview on the design rules for de novo self-assembling peptide and reviews the diverse range of bioinspired peptide nanostructures such as β-sheet and β-hairpin, α-helical and coiled coil, self-assembling short peptides and peptidomimetics, collagen-based and elastin-like peptides, silk peptides, peptide amphiphiles, peptides co-polymers and others. The book also covers the wide variety of responsive and functional biomaterials that have been innovated based on those nanostructures for various applications ranging from tissue engineering, therapeutics and drug delivery to antimicrobial nanomaterials and biosensors. Finally, the book also discusses the peptide bionanomaterials global market and the future of the emerging industry. Chapter

Self-Assembly of Peptides, Peptoids, Sugars, & Dendrimers LAP Lambert Academic Publishing

The self-organization of bionanostructures into well-defined functional machineries found in nature has been a priceless source of ideas for researchers. The molecules of life, proteins, DNA, RNA, etc., as well as the structures and forms that these molecules assume serve as rich sources of ideas for scientists or engineers who are interested in developing bio-inspired materials for innovations in biomedical fields. In nature, molecular self-assembly is a process by which complex three-dimensional structures with well-defined functions are constructed, starting from simple building blocks such as proteins and peptides. This book introduces readers to the theory and mechanisms of peptide self-assembly processes. The authors present the more common peptide self-assembled building blocks and discuss how researchers from different fields can apply self-assembling principles to bionanotechnology applications. The advantages and challenges are mentioned together with examples that reflect the state of the art of the use of self-assembled peptide building blocks in nanotechnology.

Self-assembling Cyclic D, L-peptide Nanotubes as Synthetic Transmembrane Channels from Chemical, Biological and

Practical Perspectives CRC Press
One ofthe major drivers in biological research is the establishment ofstructures and functions of the 50,000 or so proteins in our bodies. Each has a characteristic- dimensional structure, highly "ordered" yet "disordered"! This structure is essential for a protein's function and, significantly, it must be sustained in the competitive and complex environment of the living cell. It is now being recognised that when a cell loses control, proteins can se- assemble into more complex supermolecular structures such as the amyloid fibres and plaques associated with the pathogenesis of prion (CJD) or age-related (Alzheimer's) diseases. This is a pointer to the wider significance of the self-assembling properties of polypeptides. It has been long known that, in silk, polypeptides are assembled into- sheet structures which impart on the material its highly exploitable properties of flexibility combined with high tensile strength. But only now emerging is the recognition that peptides can Self-assemble into a wide variety of non-protein-like structures, including fibrils, fibres, tubules, sheets and monolayers. These are exciting observations and, more so, the potential for materials and medical exploitations is so wide ranging that over 80 scientists from Europe, USA, Japan and Israel. met 1-6 July 1999 in Crete, to discuss the wide-ranging implications of these novel developments. There was a spirit of excitement about the workshop indicative of an important new endeavor.

The emerging perception is that of a new class of materials set to become commercially viable early in the 21st century.

Peptide Self-assembly Springer Science & Business Media

"Self-assembling peptides have been found to be useful for their application as biomaterials. Ideally, these [beta]-sheet forming peptides can be designed with desired properties for a specific application. However, for this to be possible, further examination of [beta]-sheet self-assembling peptides and their resulting properties is required. Our early studies focused on studying the hydrophobic face of amphipathic peptides, using partial replacement of the hydrophobic face with increased hydrophobicity amino acids to alter self-assembly rates and morphologies. Further work was conducted on amphipathic [beta]-sheet peptides to study increased complexity of peptide systems with regards to chirality. The Ac-(FKFE)2-NH2 peptide was studied in the all-D and all-L structures and found to preferentially coassemble into rippled [beta]-sheets instead of self-sorting into pleated [beta]-sheets. Modifying the length of these peptides to an odd length, creating the peptide Ac-(FKFE)2F-NH2 which resulted in a different morphology of the D and L peptides independently, creating a mixture of coassembled and self-assembled peptides within the same [beta]-sheet. These studies represent a fundamentally new class of self-assembling peptides with unique mechanical and biological

properties. Finally, these types of peptides were studied for their use as cell penetrating peptides and as delivery vehicles. Use of the Ac-C(FKFE)2CG-NH2 peptide, which can be cyclized via a disulfide bond, allowed for application in cells as the reducing environment within the cell would break the disulfide bond, yielding a linear peptide that can be proteolytically cleaved. The cyclic variant of the peptide was used as a cell penetrating peptide for lungs cells and shown to be useful for noncovalent delivery of unmodified siRNA across the cell membrane, which cannot cross alone due to its negatively charged backbone. The work in this thesis provides additional understanding and complexity to self-assembling [beta]-sheet peptide systems and suggests additional applications of these materials"--Pages iv-v.

Peptide Self-Assembly Woodhead Publishing

The objective of this primer is to discuss the chemistry of self-assembly. It introduces some of the common reactions you need to know to prepare a desired molecule that can self-assemble (or various molecules that can be mixed to create a self-assembled system). The focus is on four self-assembled systems composed of peptides, peptoids, sugars, and dendrimers.

Self-assembly of Short Peptide Derivatives Springer

The promotion of highly order nanostructures is imperative and the presence of additive such as salts can influence the self-assembling structure

formed. Different salts can interact with charged amino acids, which promote crosslinking between peptides creating new tripeptide nanomaterials.

Peptide Self-assembly and Engineering Springer

In the past several decades, molecular self-assembly has emerged as one of the main themes in chemistry, biology, and materials science. This book compiles and details cutting-edge research in molecular assemblies ranging from self-organized peptide nanostructures and DNA-chromophore foldamers to supramolecular systems and metal-directed assemblies

Understanding the Mechanism of Peptide Self-assembly Springer Nature

Self-assembling biomaterials: molecular design, characterization and application in biology and medicine provides a comprehensive coverage on an emerging area of biomaterials science, spanning from conceptual designs to advanced characterization tools and applications of self-assembling biomaterials, and compiling the recent developments in the field. Molecular self-assembly, the autonomous organization of molecules, is ubiquitous in living organisms and intrinsic to biological structures and function. Not surprisingly, the exciting field of engineering artificial self-assembling biomaterials often finds inspiration in Biology. More important, materials that self-assemble speak the language of life and can be designed to seamlessly integrate with the biological environment, offering unique engineering opportunities in

bionanotechnology. The book is divided in five parts, comprising design of molecular building blocks for self-assembly; exclusive features of self-assembling biomaterials; specific methods and techniques to predict, investigate and characterize self-assembly and formed assemblies; different approaches for controlling self-assembly across multiple length scales and the nano/micro/macroscopic properties of biomaterials; diverse range of applications in biomedicine, including drug delivery, theranostics, cell culture and tissue regeneration. Written by researchers working in self-assembling biomaterials, it addresses a specific need within the Biomaterials scientific community. Explores both theoretical and practical aspects of self-assembly in biomaterials Includes a dedicated section on characterization techniques, specific for self-assembling biomaterials Examines the use of dynamic self-assembling biomaterials

Rational Peptide Design for Functional Materials Via Molecular Self-assembly

"Amyloid is associated with protein pathologies such as Alzheimer's disease, Parkinson's Disease, Spongiform Encephalopthies (Mad Cow's Disease), as well as Type II Diabetes. In recent years, non-pathogenic functional amyloids that are conserved in normal biological processes have been identified. Short amphipathic peptides have also been designed for the development of amyloid-inspired biomaterials. Amphipathic peptide self-assembled materials have been exploited in the

development of multivalent immunostimulants, drug delivery/gene transfection vectors, and matrices for cell and tissue growth ex vivo. Despite these impressive advancements, there remain considerable gaps in our understanding of the relationship between peptide sequence, self-assembly propensity, and the resulting fibril and hydrogel properties. Insight into the principles that govern the self-assembly and hydrogelation of amphipathic peptides will facilitate the design of amyloidinspired materials with predictable structures, properties and functions. This thesis investigates the role of aromatic [pi]-[pi] and hydrophobic noncovalent interactions in the self-assembly and hydrogelation of amphipathic peptides with the general sequence Ac-(XZXZ)2-NH2. Self-assembly propensity was found to be generally dependent on peptide hydrophobicity. Although not critical for [Beta]-sheet fibril formation, aromatic [pi]-[pi] interactions influenced the formation of unique helical tape morphologies. It was also demonstrated that hydrogel rigidity correlated to the presence of aromatic amino acids. These findings contribute insight into the basic principles that promote self-assembly and hydrogelation of amphipathic [beta]-sheet peptides. The design of functional stimulus-responsive biomaterials is increasingly important. In this thesis we also designed a peptide that could be cyclized through a reversible disulfide bond. A reduction-sensitive trigger has the potential to target the intracellular

space of cells that tends to be reducing, while the extracellular space is generally oxidizing. In the cyclic form, [beta]-sheet conformation and self-assembly were inhibited. Self-assembly and hydrogelation can be triggered by addition of chemical reductants to the cyclic peptide solution. This work demonstrated that conformational constraint is a viable trigger to control amphipathic peptide self-assembly and hydrogelation"--Page iv-v.

Protein Self-Assembly

Solid-binding short peptides offer great promise as molecular building blocks in nanotechnology and nanomedicine. Some of these peptides can form self-organized nanostructures on solid surfaces due to highly specific coordination of inter-molecular forces enabled by conformational changes in the peptide. This study aims to examine how the organization of self-assembled monolayers formed by a phage display selected “wild-type” graphite binding peptide (GrBP5-WT) change with solution conditions, such as pH and ionic strength. The surface coverage and crystallinity of these peptide monolayers were shown to increase when incubated in 1mM sodium phosphate. In contrast, GrBP5-WT incubated in 1mM sodium hydroxide showed significantly decreased coverage, and no long-range-ordered structures. Zeta potential measurements of aqueous graphite powder dispersions showed a pH-dependent negative surface charge, which increased in magnitude when GrBP5-WT was added. A peptide mutant

(GrBP5-M9) was designed by replacing two carboxylate residues with polar, but non-charged, amide residues. The mutant peptide formed crystalline nanostructures on graphite, which were unaffected by changes to the ionic strength or pH, and did not contribute additional negative charge to the graphite dispersion zeta potential. This showed that a simple mutation to a phage-display selected solid-binding peptide can eliminate its sensitivity to buffer and pH changes, facilitating the formation of more predictable bio/nano interfaces towards the development more robust biosensors and bioreactors. Self-assembly of GrBP5-WT and two other mutants (M6 and M8) was also shown on a variety of different atomically-flat 2D solid substrates, including CVD graphene on copper, and exfoliated BN, MoS_2, $MoSe_2$, WS_2, and WSe_2 on SiO_2/Si. Although long-range ordered structures were shown on each substrate material, subtle differences in the patterns formed on each substrate indicate an important influence of the underlying crystal structure on the peptide nanostructure. The ready formation of ordered nanostructures opens the door for an investigation of the physical properties of number of hybrid nanomaterials. In particular, solid-binding peptides were shown to induce a molecular doping effect on the photoluminescence of single-layer $MoSe_2$ (a 2D semiconductor with a direct band-gap in the visible light spectrum). Peptide self-assembly was also found to be sensitive to the presence of polymer

residues commonly used in lithographic processing (such as PMMA). Indium microsoldering was investigated as a means to prepare electronic devices (such as graphene field-effect transistors) without contaminating the substrate.