2015 Soft Matter Summer School : Polymers in Biology

Poster Abstract Book

Introduction

Discoveries in polymer physics and chemistry impact diverse phenomena in biology. Biopolymers, special forms of polymers realized through evolution, can adopt three-dimensional native structures and reshape their conformations in response to changes in external conditions. The basic static and dynamic features of single- and many- polymer systems are central for the understanding of proteins, nucleic acids, polysaccharides, and their complexes. The overall aim of this summer school is to bring together polymer experts from diverse disciplines whose works are linked to polymer science and biology in order to promote the basic science underlying biological materials and living organisms.

The foci of the "2015 Soft Matter Summer School : Polymers in Biology" will be on the: (1) properties of a single polymer (statics and dynamics) and its response to environmental changes; (2) collective behavior of polymers. More specifically, the following topic will be covered:

1. Basic polymer theories and simulations.
2. Mechanics of nucleic acids.
3. From DNA to higher order complexes and the chromosome.
3. Protein folding.
4. Intrinsically disordered proteins
5. Effects of crowded environment on biopolymers.
6. Cytoskeletal filaments
7. Glycomaterials.
8. Active materials.

The 2015 Summer School will be organized by the Korea Institute of Advanced Study (KIAS), Institute for basic science (IBS) and ICMR (International Center for Materials Research, UCSB). It will begin with two-day pre-school workshop, in which all the participants will have a chance to present their current work and be followed by the body of the school. The 12 invited speakers will each deliver a 4-hour mini-course on polymer science and their applications to biology. The initial few hours of each mini-course will be devoted to the fundamental, textbook level introduction to basic concepts.

Lecturers

- M.C. Choi (KAIST) : Structures and interactions of microtubules and microtubule-associated-molecules
- Kamil Godula (UCSD)
- Multiscale studies of macromolecular systems: concepts and applications
- Jooyoung Lee (KIAS) : Protein Structure Prediction and Global Optimization
- Seok-Cheol Hong (Korea Univ.) : DNA mechanics and structural diversity of DNA
- Fyl Pincus (UCSB)
- Jennifer Ross (Univ. Mass)
- Omar Saleh (UCSB) :
  1) Biopolymers in tension
  2) Electrostatics of flexible biopolymers
- Helmut Schiessel (Univ. Leiden) : Chromatin: a multi-scale jigsaw puzzle in biological physics
- Ben Schuler (Univ. Zurich) : Single-molecule spectroscopy of unfolded and intrinsically disordered proteins
- Mitsuhiro Shibayama (Univ. Tokyo)
  - Neutron and Rheology
  1. Structural Analyses of Polymers by Small Angle Neutron Scattering
  2. Contrast Variation SANS -The basics and applications
  3. Rheo-SANS Studies on Structure Evolution in Polymer-particle Aqueous Solutions.
- Dave Thirumalai (Univ. Maryland)
- Megan Valentine (UCSB) : Biopolymer network mechanics
  1. Microrheology, with a strong emphasis on biopolymers.
  2. Cytoskeletal mechanics, with lots of detail on instrumentation and experiments.

Organizers

- Changbong Hyeon (KIAS)
- Mahnwon Kim (GIST)
- Hyuk Kyu Pak (UNIST/IBS)
- Fyl Pincus (UCSB)

Program Schedule

2015 Soft Matter Summer School: Polymers in Biology

1st WEEK

Time	June 21 Sun	June 22 Mon	June 23 Tue	June 24 Wed	June 25 Thurs	June 26 Fri	June 27 Sat
8:00	ARRIVAL	BREAKFAST					EXCURSION / FREE TIME
8:30		Preworkshop	Pincus	Saleh	Schuler	Schiessel	
			Pincus	Saleh	Schuler	Schiessel	
10:20			Break				
10:40			Hong	Schuler	Choi	Hong	
			Hong	Schuler	Choi	Hong	
12:30		LUNCH					
13:30		Preworkshop	Poster Session				
15:00						Saleh	
16:00		Choi	Kremer	Schiessel	Kremer	Saleh	
17:00		Choi	Kremer	Schiessel	Kremer		
17:50	Preworkshop	DINNER / GROUP STUDY / DISCUSSION				BANQUET	
20:00							

2nd WEEK

Time	June 28 Sun	June 29 Mon	June 30 Tue	July 1 Wed	July 2 Thurs	July 3 Fri
8:00	FREE TIME	BREAKFAST				
8:30		Lee	Ross	Thirumalai	Valentine	Group Presentation
		Lee	Ross	Thirumalai	Valentine	
10:20		BREAK				
10:40		Godula	Lee	Godula	Shibayama	
		Godula	Lee	Godula	Shibayama	
12:30		LUNCH				
13:30		GROUP STUDY/DISCUSSION				CLOSING DISCUSSION
16:00		Thirumalai	Valentine	Shibayama	Ross	
		Thirumalai	Valentine	Shibayama	Ross	
17:50		DINNER / GROUP STUDY / DISCUSSION				FAREWELL PARTY
20:00						

List of Posters

1. **Quantifying the ion atmosphere of unfolded, random-coil nucleic acids**
   - David Jacobson
2. **Electrostatic effects on hyaluronic acid elastic behavior**
   - John Berezney
3. **Effects of Counterion Condensation on the Electrophoresis of DNA**
   - Pyeong Jun Park
4. **Destabilizationof i-motif by Sub-molar Concentrations of a Monovalent Cation**
   - SungEun Kim
5. **The effect of cisplatin on nucleosomal DNA**
   - Hyeon-Min Moon
6. **Sequence-specific DNA looping by mitochondrial transcription factor A (TFAM)**
   - Divakaran Murugesapillai
7. **Elastic correlations in di-nucleosome structure**
   - Fatemeh Khodabandeh
8. **Tension-induced Binding of Semiflexible Biopolymers**
   - Panayotis Benetatos
9. **Cantilevered PEDOT Fibers for Sub-Celluar Force Measurement**
   - Govind Paneru
10. **Polyelectrolyte Brushes in Multivalent Salt Solutions: Bridging Effects**
    - Blair Kathryn Brettmann
11. **Study on the folding of a group II intron ribozyme – The effects of crowding agents and mutations**
    - Erica Fiorini
12. **Analyzing dynamic heterogeneity in single molecule experiment**
    - Wonseok Hwang

13. **Simulation of FRET Dyes with Native Structure-based Models**
    - Ines Reinartz
14. **Mechanical control of folding pathway of DNA origami structures**
    - Kipom Kim
15. **Velocity distribution of Kinesin is bimodal under load**
    - Huong Vu
16. **Following the steps of dynein: Explaining dynein's step size distribution using analytical models**
    - Yonathan Goldtzvik
17. **Unfolding Mechanism of Myosin VI Proximal Tail**
    - Mauro L. Mugnai
18. **LINE1 retrotransposition in human cells requires rapid ORF1p oligomerization**
    - M. Nabuan Naufer
19. **Implementing a Model Force Field for tRNA Translocation through a Nanopore**
    - Prasad Bandarkar
20. **Structure and dynamics of intrinsically disordered linkers in multidomain proteins**
    - Sebastian L. B. König
21. **Understanding structural mechanism of β_2-adrenergic receptor with water dynamics**
    - Songmi Kim
22. **New Materials For Gene Delivery In Difficult-To-Transfect Cell Lines**
    - Spencer Brucks
23. **Study on determining the average size and structures of nanoparticles**
    - Sujan Dhungana

24. **Biosorption of zinc (II) metal onto raw and modified coconut husks and tea waste**
    - Surendra K. Gautam
25. **Synthesis and characterization of nanocrystalline zinc selenide**
    - Dipak Koirala
26. **Dynamics of Water Molecules Binding to Magnesium or Sodium Ions**
    - Yuno Lee
27. **Curvature Asymmetry in Water Coalescence**
    - Su Jin Lim
28. **Self-propelled motion of reactive droplets**
    - In Gyu Hwang
29. **Slowly drying of dense coffee droplets**
    - Jin Young Kim
30. **Measuring mechanical properties of live cells and artificial lipid vesicles reinforced by ECM network**
    - Serin Lee
31. **Formation of ECM-binding liposome; ECM Cellular Delivery**
    - Sojeong Nam
32. **Gelation-induced crack prevention in colloidal films**
    - Seul-a Ryu
33. **Revisiting the fundamental origin of aromatic interaction**
    - Hankyul Lee
34. **Recapitulation of Cell Surface Glycan Presentations using Multivalent Glycomaterials for Study of Influenza A Virus Specificity**
    - Chris Fisher
35. **Single molecule Raman scattering spectroscopy under high pressure**
    - Yuanxi Fu

36. Microrheology of semi-dilute aqueous solutions of polyethylene oxide probed by an optically trapped micro-bead

- Chong Shen

[P1] Quantifying the ion atmosphere of unfolded, random-coil nucleic acids

David Jacobson

University of California, Santa Barbara

Much of the biological function of nucleic acids (NAs) is imparted by the formation of helices through Watson-Crick base pairing. Since the NAs are strongly charged, a physical understanding of this simplest instance of folding must include the effects of electrostatics, and its screening by ions in solution, on both the folded and unfolded states. The relevant parameter for describing these ion interactions is the ion excess: the number of ions present near the NA in excess of the bulk concentration. The ion excess associated with the folded, helical state is well described by the Poisson-Boltzmann (PB) equation; however, the ion excess of the unfolded, random-coil state is less well understood. Here, we quantify the ion atmosphere of the random-coil state using two independent methods: a direct method, employing equilibrium dialysis read out by atomic emission spectroscopy (D-AES), and an indirect method, in which we start with the helix result from PB theory and then subtract the ions released as the helix is mechanically unfolded. Both methods show a broad regime in which the ion excess of the random-coil state is independent of bulk salt concentration, a result we attribute to the competing effects of bulk charge screening and salt-dependent structural compaction.

[P2] Electrostatic effects on hyaluronic acid elastic behavior

John Berezney, Omar Saleh
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University of California, Santa Barbara

Hyaluronic acid (HA) is a polyelectrolyte found in both prokaryotic and eukaryotic organisms. Its conformational properties are particularly important for defining the mechanics of the extracellular matrix. To investigate the relation between electrostatics and chain conformation, we perform single molecule experiments on HA using magnetic tweezers to measure the extension as a function of applied tension and ionic strength. Over a limited range of low ionic strength (<10 mM), we observe two regimes of elastic behavior, consistent with good-solvent conditions: At low forces, HA extension grows as a power-law with force, with an exponent associated with swollen chain behavior. At higher forces, HA transitions to a less-elastic behavior that deviates from ideal-polymer predictions. In these salt conditions, HA acts as a chain of Debye-length scale blobs with anomalous structure, analogous to that seen previously for single-stranded nucleic acids (ssNAs). Above 10 mM salt, HA's elastic response fundamentally changes to a single elastic behavior across all forces that is well-described by the ideal WLC (Marko-Siggia). In contrast to results for ssNAs, HA's ideal behavior is robust across a wide range of monovalent salt (100 mM-5 M). We attribute this robustness to non-electrostatic effects on HA structure, particularly its intrinsic stiffness and hydrophilicity.

[P3] Effects of Counterion Condensation on the Electrophoresis of DNA

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We perform the molecular dynamics simulation of charged polymers under external electric fields, where explicit counterions and additional salt ions are taken into account. To incorporate the hydrodynamic effects, we use the multiparticle collision dynamics scheme via the stochastic rotation dynamics, and the canonical thermostat is employed to maintain the temperature of the system. Our result shows that salt ions not only screen out the electrostatic interaction among the charged polymer and counterions, but also they take part in the counterion condensation significantly. We show the mobility of the charged polymer under electric fields as a function of the molecular weight of the polymer and salt concentration, which are in agreements with experimental observations.

[P4] Destabilizationof i-motif by Sub-molar Concentrations of a Monovalent Cation

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**** School of Computational Sciences, Korea Institute for Advanced Study, Seoul130-722, Korea**
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Wediscovered that high concentration of lithium ions, in contrast to othermonovalent cations, destabilizes a cytosine-quadruplex called i-motif bypromoting its unfolding, not hindering its folding. We obtained such kineticinformation by a new analysis scheme named HaRP. The unusual destabilization bylithium cations can be attributed to the small size of a lithium ion, which candisrupt hydrogen bonding between cytosines in i-motif.

[P5] The effect of cisplatin on nucleosomal DNA

Hyeon-Min MOON[1], Jin-Sung PARK[2], Ilbuem LEE[1], Nam-Kyung LEE[3], Ji-Joon SONG[4], kyoung J. LEE[1] Seok-Cheol HONG[1]

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[3]Department of Physics, Sejong Univ. [4]Department of Biological Sciences, KAIST

The hallmark of cancerous cells is their perpetual cell division, and they thus push and replace intact normal cells. Chemotherapeutic agents help to cure cancers by introducing apoptosis in the affected cells. Cisplatin, one of the most effective cytotoxic agents and the first-generation platinum-based anti-cancer drugs, has been widely used in cancer chemotherapy for decades. The well-known mechanism of cisplatin is that the drug binds and kinds DNA via cross linking and the bound DNA cannot be repaired by normal DNA repair pathways. As a result, cells undergo apoptosis. DNA exists in the form of nucleosome inside cells. Therefore, the interaction between cisplatin and nucleosomes is crucial for understanding the anti-cancer effect of cisplatin. To study this at single-molecule level, we reconstitute nucleosomes on a single DNA tether molecule under physiological ionic condition by using a histone chaperone called NAP1. With the reconstituted chromatin, we observe that cisplatin fastens chromatin, which can interfere with normal DNA metabolism. This observation shed new light on the molecular mechanism of the anti-cancer effect of cisplatin.

[P6] Sequence-specific DNA looping by mitochondrial transcription factor A (TFAM)

Divakaran Murugesapillai[1], Maria F. Lodeiro[2], L. James Maher III[3], Craig E. Cameron[2], and Mark C. Williams[1]

[1] Northeastern University, Department of Physics, Boston, MA 02115, USA;[2] Pennsylvania State University, Department of Biochemistry and Molecular Biology, University Park, PA 16802, USA;[3] Mayo Clinic College of Medicine, Department of Biochemistry and Molecular Biology, Rochester, MN 55905, USA;

Mitochondrial transcription factor A (TFAM) is an abundant human mitochondrial High Mobility Group Box (HMGB) protein. Similar to several human nuclear HMGB proteins, TFAM has two HMGB domains that facilitate DNA binding and bending [1-3]. TFAM is an architectural protein known to play an essential role in shaping and maintaining the mitochondrial DNA (mtDNA). It is also known to be involved in regulating mitochondrial transcription. Sequence-specific binding of TFAM to DNA upstream of the light-strand promoter (LSP) leads to bending that correlates with transactivation of this promoter. The role for TFAM and corresponding mechanism at other promoters is likely different than observed at LSP [4]. For example, transcription from HSP1 uses far more upstream sequence than required at LSP. Here we use a dual promoter construct containing both LSP, HSP1 and the natural inter-promoter region to understand the role of the IPR on transcription. We show that the IPR contributes to TFAM transactivation of HSP1. Removal of the carboxy-terminal tail of TFAM (TFAM-ΔCT26) leads to a complete loss of transactivation of HSP1 with only minimal effects on LSP. By using atomic force microscopy (AFM), we observe that TFAM preferentially binds to the IPR. In addition, we find that at low concentrations of TFAM, this binding leads to formation of DNA loops in a region consistent with the IPR. Interestingly, under the same conditions, TFAM-ΔCT26 fails to produce DNA loops. Importantly, at higher concentration both TFAM and TFAM-ΔCT26 are equally efficient at DNA compaction. Taken together, our results are consistent with sequence-specific DNA looping contributing to TFAM transactivation of HSP1, suggesting that unique mechanisms are employed for TFAM-dependent transcription at LSP and HSP1.

References

1. Ngo, H.B., G.A. Lovely, R. Phillips, and D.C. Chan, *Distinct structural features of TFAM drive mitochondrial DNA packaging versus transcriptional activation.* Nat Commun, 2014. **5**: p. 3077.
2. Rubio-Cosials, A., J.F. Sidow, N. Jimenez-Menendez, P. Fernandez-Millan, J. Montoya, H.T. Jacobs, M. Coll, P. Bernado, and M. Sola, *Human mitochondrial transcription factor A induces a U-turn structure in the light strand promoter.* Nat

Struct Mol Biol, 2011. **18**: p. 1281-9.

3. Ngo, H.B., J.T. Kaiser, and D.C. Chan, *The mitochondrial transcription and packaging factor Tfam imposes a U-turn on mitochondrial DNA.* Nat Struct Mol Biol, 2011. **18**: p. 1290-6.
4. Lodeiro, M.F., A. Uchida, M. Bestwick, I.M. Moustafa, J.J. Arnold, G.S. Shadel, and C.E. Cameron, *Transcription from the second heavy-strand promoter of human mtDNA is repressed by transcription factor A in vitro.* Proc Natl Acad Sci U S A, 2012. **109**: p. 6513-8.

[P7] Elastic correlations in di-nucleosome structure

Fatemeh Khodabandeh

Institute for Advanced Studies in Basic Sciences (IASBS)

We study a di-nucleosome system under tension using a theoretical model that takes into account the nucleosomal geometry and DNA elasticity. Using a numerical method and energy minimization in the phase space of the two nucleosomes, we find the structure of this system. We show that the energy and the spatial structure of a di-nucleosome system is independent of the DNA linker length.

[P8] Tension-induced Binding of Semiflexible Biopolymers

Panayotis Benetatos

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We investigate theoretically the effect of polymer tension on the collective behaviour of reversible cross-links. We use a model of two parallel-aligned, weakly-bending wormlike chains with a regularly spaced sequence of binding sites subjected to a tensile force. Reversible cross-links attach and detach at the binding sites with an affinity controlled by a chemical potential. In a mean-field approach, we calculate the free energy of the system and we show the emergence of a free energy barrier which controls the reversible (un)binding. The tension affects the conformational entropy of the chains which competes with the binding energy of the cross-links. This competition gives rise to a sudden increase in the fraction of bound sites as the polymer tension increases. The force-induced first-order transition in the number of cross-links implies a sudden force-induced stiffening of the effective stretching modulus of the polymers. This mechanism may be relevant to the formation and stress-induced strengthening of stress fibers in the cytoskeleton.

[P9] Cantilevered PEDOT Fibers for Sub-Celluar Force Measurement

Govind Paneru
IBS Center for Soft and Living Matter, UNIST

Maneuverable, high aspect ratio poly(3,4 ethylene dioxythiophene) (PEDOT) fibers are fabricated for use as cellular force sensors. These fibers are capable of probing individual sub-micron sized adhesive contact sites without forming unintentional secondary contacts to the cell. The length and diameter of a fiber are user controlled, and consequently their spring constants. The spring constants of these fibers were measured directly using atomic force microscopy (AFM). The AFM measurements agree with the spring constant determinations based on the resonance vibration of the fibers, which is more convenient method. These fibers are employed to characterize the time dependent forces exerted at adhesive contacts between apical pseudopods of highly migratory D. discoideum cells and the PEDOT fibers.

[P10] Polyelectrolyte Brushes in Multivalent Salt Solutions: Bridging Effects

Blair Kathryn Brettmann

The Institute for Molecular Engineering, The University of Chicago

Polyelectrolyte brushes have attracted a great deal of interest in recent years for technological applications ranging from colloidal stabilization (to lubrication, as well as serving as models for biological polymers such as DNA in crowded environments that mimic cellular microenvironments. Of particular interest is the distance the polymer chains extend from the surface, as this provides much of the functionality of these materials. Electrostatic and excluded volume interactions between chain segments and osmotic pressure from counter-ions in the brush volume counteract the polymer chain elasticity to result in extension normal to the tethering surface. This behavior is well understood both theoretically and experimentally for polyelectrolyte brushes in the presence of monovalent counter-ions. In the presence of multivalent counter-ions, however, the brush has been shown to undergo a sharp collapse to a significantly lower brush height with increasing multivalent ion concentrations, which is expected to be caused in part by bridging of the polyelectrolyte chains by the multivalent ions. We expand current models of polyelectrolyte brushes to include treatment of bridging and its contribution to brush collapse. Using an energy balance represented by the sum of electrostatic, polymeric and entropic mean-field terms, we introduce an additional phenomenological mean-field term for the attractive interaction between adjacent polyelectrolyte chains to account for the bridging effect. The free energy is minimized with respect to the counter-ion populations and the brush height. In agreement with experimental observations, increasing the concentration of multivalent ions leads to a sharp collapse of the polyelectrolyte brush height.

[P11] Study on the folding of a group II intron ribozyme – The effects of crowding agents and mutations

Erica Fiorini, Richard Börner and Roland K.O. Sigel

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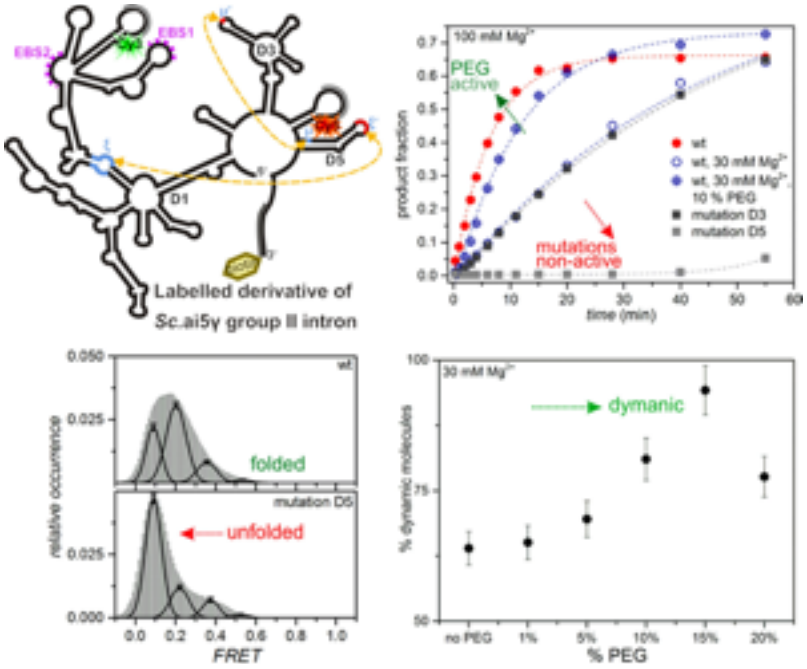
Group II introns are among the largest ribozymes known. Their structural analysis suggests that they have evolved into ribonucleoproteins generating the eukaryotic nuclear spliceosome. They are found in the genome of bacteria, plants and lower eukaryotes [1]. These self-splicing ribozymes are active upon formation of specific long-range tertiary interactions that define a precise conformation influenced by metal ions [2,3]. In particular, group II intron ribozymes are known to require a high Mg^{2+} concentration for show folding and function *in vitro*. In contrast, *in vivo* conditions are characterized by a highly crowded cellular environment and much lower ion concentration. Nowadays, molecular crowding agents, like poly(ethylene)glycol (PEG), are a widespread tool to mimic cellular crowding and thus, to reach near physiological conditions [4].

We study the folding pathway of a truncated but active Sc.ai5γ group II intron through point mutations in the RNA sequence in positions essential for inter-domain docking and the effect of PEG on the folding [3]. We combined bulk activity assays and single-molecule Förster Resonance Energy Transfer (smFRET) experiments to test if the presence of a crowding agent can stabilize the folding of this ribozyme at a lower concentration of Mg^{2+} and which mutation causes specific changes in the folding.

In particular smFRET allowed us to quantify the differences in the relative population of a certain conformation attributed for splicing activity. For example, a clear shift towards the unfolded conformations is detected when the catalytic domain (D5) is mutated [5]. Instead, under the influence of a crowding agent, the population of higher FRET states, corresponding to the native state, is shifted towards lower concentrations of Mg^{2+}. In addition, activity assays in the presence of PEG reveal that the concentration of Mg^{2+} required to obtain the fully active ribozyme is reduced by more the 50% [6].

As a result, molecular crowding helps the ribozyme to reach a more packed and consequently native fold near physiological conditions, explaining the effect of the packed milieu *in vivo*.

From the mutated constructs, we can assign a change in conformation/FRET state to a particular event in the folding, providing us with a deeper understanding of the actual active state. Targeting specific domains, in particular single motifs, drastically decreases the activity making group II introns a possible target for drugs. Furthermore, their capability to reinsert into the genome may ultimately be applicable for gene therapy.



[1] Pyle A.M. *Crit. Rev. Biochem. Mol. Biol.*, 2010, 45, 215-232.

[2] Sigel R. K. O. *Eur. J. Inorg. Chem.*, 2005, 12, 2281-2292.

[3] Steiner M., Karunatilaka K., Sigel R.K.O. and Rueda D. *Proc. Natl. Acad. Sci. USA*, 2008, 105, 13853–13858.

[4] Nakano S., Miyoshi D. and Sugimoto N. *Chem. Rev.,* 2014, 114, 2733-2758

[5] König S.L.B., Hadzic M., Fiorini E., Börner R., Kowerko D., Blanckenhorn W.U. and Sigel R.K.O. *PLoS ONE*, 2013, 8:e84157.

[6] Fiorini E., Börner R. and Sigel R. K.O. *Chimia*, 2015, 69, 207-212; Fiorini E., Paudel B., Börner R., Rueda D., Sigel R.K.O., *in preparation.*

[P12] Analyzing dynamic heterogeneity in single molecule experiment

Wonseok Hwang,[1] Il-Buem Lee,[2] Seok-Cheol Hong,[2] and Changbong Hyeon[1]

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Markov chain is ubiquitous in many biological models. For example reversible conformational dynamics of biomolecules are often modeled as homogeneous Markov process of which the kinetic rates of their dynamics remain constant along the time. The rationals for using homogeneous Markov chain is based on the implicit assumption that same biomolecules are all folded into a unique functionally competent folded-state. However recent single molecule experiments have revealed that there are persistent molecule-to-molecule variations in their conformational kinetic rates indicating that there could be several functionally competent folded-states due to trapping of molecule in local minimum of their rugged folding-energy landscape. For such system, it maybe natural to think that the interconversion between folded-states can happen along the time depending on the scale of energy barriers. In this case, biomolecule which initially has conformational dynamics with certain time scale can show slower/faster conformational dynamics at a later time demonstrating dynamic heterogeneity. Indeed, we recently found that the triplex formation dynamics of H-DNA shows dynamic heterogeneity. Conventional modeling using homogeneous Markov process cannot be used to describe the system with dynamic heterogeneity without risk of losing information.

Here we have developed the method to analyze dynamic heterogeneity in single molecule data containing information about conformational dynamics of individual molecules in the form of 1-D time trajectories. Our method can test quantitatively the existence of dynamic heterogeneity in each trajectory and can separate it into the set of homogeneous trajectories. Our method also can estimate how many homogeneous states are mixed in the individual trajectories and can estimate transition rates between homogeneous states as well as the kinetic rates of conformational dynamics of each homogeneous state. We used our method to analyze the duplex-triplex transition dynamics of H-DNA.

[P13] Simulation of FRET Dyes with Native Structure-based Models

Ines Reinartz[1,2], Claude Sinner[1,2], Benjamin Lutz[1,2], and Alexander Schug[1]

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Forster Resonance Energy Transfer (FRET) experiments can provide valuable informa- tion about protein dynamics. By measuring the energy transfer depending on the distance between a donor and an acceptor fluorophore it is possible to observe different protein conformations. The energy transfer efficiency not only depends on the distance but also on the mutual orientation of the dyes, which both can be gained from atomistic simulations [1].

We integrate FRET fluorophores with the help of eSBMTools [2, 3] into an all-atom structure based model (SBM) to improve the interpretation of FRET measurements via FRET efficiency distributions from our simulations.

[1] Hoefling et al., PLoS ONE 6, 2011
[2] Lutz et al., Bioinformatics 29, 2013
[3] http://sourceforge.net/projects/esbmtools/

[P14] Mechanical control of folding pathway of DNA origami structures

Kipom Kim[1] , Wooli Bae[2], Changbong Hyeon[3], and Tae-Young Yoon[1,2]

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Despite the recent development in DNA origami design, its folding yet relies on thermal or chemical annealing methods. Since the folding landscape involved in such annealing methods is rugged, the whole folding process typically takes tens of hours. We present a new method for DNA origami folding, where folding pathway is controlled by mechanical forces. Using single molecule force spectroscopy technique - magnetic tweezers, we stretch a scaffold DNA with 5 pN of force to remove its secondary structures and induce efficient hybridization with staple strands. And then, the force is subsequently quenched to 0 pN. Since then, the scaffold DNA starts to fold into nanostructure through displacement between the bound staple strands. Because each process in the folding pathway is free from kinetic traps, the whole folding process finishes within 10 minutes.

[P15] Velocity distribution of Kinesin is bimodal under load

Huong Vu
University of Maryland, College Park

Understanding the distribution of velocities of identical motors as they walk along polar tracks is important in deciphering their locomotion mechanism. We created a three parameter kinetic model to describe the velocity and run-length distributions (P(v) and P(n)) of generic molecular motors that step (forward and backward) on a track and have finite processivity, under a resistive load. Remarkably, our theory explains Kinesin-1 data, both P(n) and P(v), very well at zero force with a single parameter fitting. When extended to predict the behavior of Kinesin-1 velocity distributions under non-zero loads, the theory makes two interesting predictions. One is that the P(v) is non-Gaussian and the other is a bimodal structure in P(v). The bimodal structure, a feature that remains even with a finite step-size distribution, is a direct consequence of the discrete step-size of Kinesin-1. Although we analyze only Kinesin-1 data, our results are general and should hold for any processive motor, which walks on a polar track with a discrete step-size.

[P16] Following the steps of dynein: Explaining dynein's step size distribution using analytical models

Yonathan Goldtzvik

University of Maryland, College Park

Cytoskeletal motors such as kinesins, myosins, and dyneins are tools used by living cells to convert chemical energy into mechanical work. They participate in a wide selection of processes including transportation of cargo along microtubules, muscle cell contraction, and chromosomal segregation. It is therefore important to understand the mechanisms with which these motors operate. While motors belonging to the kinesin and myosin families seem to advance along microtubules/actin filaments with a more or less fixed step size, dyneins exhibit a wide distribution of step sizes including steps backwards. In order to explain this step size variation we use a simple mechanical model of the dynein dimer which can be solved analytically. By combining this mechanical model with a Markov chain approach we are able to approximately reproduce the step size distribution of dynein as well as other properties such as the motor's velocity, run length and mean dwell time.

[P17] Unfolding Mechanism of Myosin VI Proximal Tail

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Like myosin V, myosin VI dimers walks on actin filaments, but in the opposite direction. The size of a myosin dimer step depends on the length of the lever arm. In myosin V the lever arm is made of six calmodulin (CaM)-binding domains. Myosin VI average step size is comparable to myosin V, despite it has only one CaM-binding domain. Therefore, some other part of the protein must extend the lever arm to compensate for the gap. Experimental evidence suggests that two domains of myosin VI tail might be involved in the extension: the proximal tail (PT), and the medial tail (MT). PT is a helical bundle, while MT is a single alpha-helix characterized by a ER/K sequence (four E residues followed by four R/K residues). It was suggested that the MT is involved in formation of the dimer, and that upon dimerization the PT unfolds to contribute to the size of the swing. The question is: what is the unfolding mechanism? What are the interactions that trigger the unfolding?

Here, I discuss the study that I intend to perform with a coarse grained, native-structure based self-organized polymer (SOP) model to address this question. I present preliminary simulations of PT and MT thermal unfolding, aimed at the comparison with the circular dichroism spectra.

[P18] LINE1 retrotransposition in human cells requires rapid ORF1p oligomerization

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ORF1 protein (ORF1p) is encoded by the long interspersed nuclear element-1 (LINE1) retrotransposon. LINE1 replicates by converting its transcript into genomic DNA, a mechanism that can also similarly process some host gene transcripts. LINE1 activity has thereby greatly expanded mammalian genomes during evolution and it causes variety of genetic changes in the modern human genome. The role of human ORF1p (hORF1p) in LINE1 retrotransposition is largely unknown, although it presumably involves its nucleic acid chaperone activity and its ability to oligomerize on nucleic acids. To better understand the molecular mechanism of hORF1p in LINE1-retrotransposition, we developed a novel method to characterize single-stranded DNA (ssDNA)-hORF1p interactions using single molecule stretching with optical tweezers. Here we study three hORF1p variants; the modern wild type, an ancestral wild type and a hybrid in which nine residues in the coiled coil domain of the modern wild type is substituted with the corresponding ancestral residues. These hORF1p variants are equally stable in the cell and indistinguishable as nucleic acid chaperones. Remarkably, the hybrid variant is completely dead in retrotransposition while both wild type variants are completely active. We characterized three distinct ssDNA binding kinetics for all three hORF1p variants. A fast kinetic fraction characterized by association and dissociation on a timescale of seconds, an intermediate fraction with a timescale of greater than one minute, which characterizes dissociation of the protein after the stretching force on DNA is released, and a slow fraction with dissociation on a timescale of tens of minutes. The fast fractions of all variants are converted to intermediate and slow fractions with time, consistent with protein oligomerization. However, the oligomerization rate on ssDNA for the hybrid is orders of magnitude less than that of the wild types. This significant difference in hybrid protein oligomerization provides a compelling explanation for its inability to facilitate retrotransposition, suggesting that rapid oligomerization is critical for LINE1 retrotransposition.

[P19] Implementing a Model Force Field for tRNA Translocation through a Nanopore

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The fidelity of mRNA translation depends not only upon the codon -anticodon pairing between the mRNA and the tRNA but also upon the structure of the tRNA far from the anticodon site. Therefore many experimental techniques aim to probe the conformational properties of different tRNA molecules. Electrophoretic translocation of biomolecules through a solid-state nanopore represents a label-free single molecule technique that may be used to identify distinct structural features of different types of molecules. This tool has been used extensively for detecting and distinguishing single stranded DNA and double stranded DNA. Recent investigations have attempted to distinguish individual tRNA molecules from each other by characterizing pore translocation times and blockage currents. These nanopores are large enough to accommodate the anticodon loop while being narrow enough to not allow the passage of the molecule without deformation from the traditional L-shaped structure. We apply MD simulations using a simplified structure-based energetics model of the molecule to study the structural changes in tRNA during translocation. We have implemented a simplified force-field between the nanopore walls and the molecule to mimic the steric effect of these walls. Through the use of umbrella sampling we calculated the free energy barrier for different tRNA species and have identified the residues that undergo partial unfolding during translocation. These results provide a structural/energetic interpretation of current experiments, which can help help one refine methods for single-molecule detection using nanopores.

[P20] Structure and dynamics of intrinsically disordered linkers in multidomain proteins

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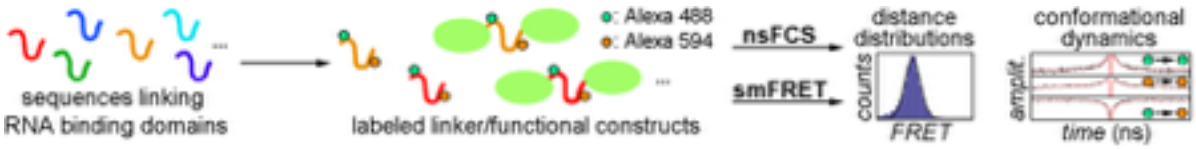
Multidomain proteins occupy nearly half of all proteomes and typically consist of several folded domains that are spaced via flexible linkers.[1] The sequence of these linkers is often highly conserved, suggesting biological importance. Little is known, however, about the structural interplay of folded and unfolded regions in multidomain proteins and the consequences for the function of the protein as a whole. We use single-molecule methods to investigate the effect of the amino acid sequence on the structure and dynamics of intrinsically disordered linkers in the presence and absence of neighbouring folded domains.

We selected a series of naturally occurring linker sequences spacing RNA binding domains. Single-molecule Förster resonance energy transfer (smFRET) and nanosecond fluorescence correlation spectroscopy (nsFCS) were used to characterise the structure and conformational dynamics of the different sequences in the presence and absence of two adjacent folded double-stranded RNA-binding domains. We intend to use concepts from polymer physics to relate the differences in distance distributions and chain dynamics to the sequence composition of the linkers and the conformational constraints originating from the domains.



[1] Han JH, Batey S, Nickson AA, Teichmann SA, Clarke J (2007) The folding and evolution of multidomain proteins. *Nat. Mol. Cell Biol.* 8:319-330

[P21] Understanding structural mechanism of β_2-adrenergic receptor with water dynamics

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G protein-coupled receptors (GPCRs) are membrane proteins and responsible for various cellular responses by signal molecules including hormones, odorants, neuro- transmitter and other factors. The conformational change of the GPCR is induced by signal molecule binding, which allows to transmit signals from extracellular to intracel- lular across membrane. Several GPCR crystal structures revealed that the activation of GPCRs is mediated by structural water molecules. To understand structural mecha- nism focused on water molecules within β_2-adrenergic receptor (β_2AR), we constructed systems for different states including inverse agonist bound-β_2AR and apo as inactive state, and agonist bound-β_2AR with and without Gα, and apo, as active state. We have performed 1μs all-atom MD simulation for each system in membrane environment. The dynamics of water molecules in β_2AR and structural analysis have been carried out by time correlation function of contacts between residue and water molecules and by calculating the water penetration.

[P22] New Materials For Gene Delivery In Difficult-To-Transfect Cell Lines

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Polyelectrolytes hold potential to be transformative in applications as diverse as energy storage and therapeutics. Materials that possess both inherent compositional modularity and ready accessibility via robust and scalable synthetic pathways are of particular import to the field. Thus far, development of cationic polyelectrolytes has been limited to a few monomeric functionalities, such as imidazolium, ammonium, and iminium, which bear formal charge on heteroatoms and lack broad modularity. The cyclopropenium ion could address these challenges, while offering a highly unique structural architecture and electronic properties. This presentation will focus on cyclopropenium-based nanoparticles to transfect gastric carcinomas – cancer cells that have not been previously transfected. We show that we can synthesize surface-charged nanoparticles of tunable size via surfactant-free emulsion polymerization. Moreover, we discuss a label-free imaging technique to track these materials comprising only styrene and cyclopropenium ion monomers. Our results have broad implications in biotechnology for studying mechanisms of cell transfection and function in addition to novel therapeutic applications.

[P23] Study on determining the average size and structures of nanoparticles

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Semiconductors are the foundation of modern electronics, including transistors, solar cells, light emitting diodes (LEDs), quantum dots etc. Researchers have studied semiconductor nanoparticles intensely and have developed them for broad applications in solar energy conversion, optoelectronic devices, molecular and cellular imaging, ultrasensitive detection, targeted therapy etc. All applications are size dependent and their crystalline structures play vital role. Synthesizing nano-sized semiconductor particles and stabilizing structure is always challenging. Group II-VI semiconductor NPs can be synthesized by various ways as chemical deposition, biomimic, sol-gel, microemulsion, microwave irradiation, spray pyrolysis etc. The crystalline structure with phase purity can be settled using XRD data and SAED pattern. The average particle sizes are determined with the help of UV spectra and XRD data which also could be confirmed from TEM images.

Keywords: Semiconductor NPs, X-ray Diffraction (XRD), UV spectra, Transmission Electron Microscopy (TEM)

[P24] Biosorption of zinc (II) metal onto raw and modified coconut husks and tea waste

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Biosorption is potentially an attractive technology for treatment of waste water for retaining heavy metals from dilute solutions. Several researches' in environmental biotechnology have shown that many biosorbents present in our environment have the capacity to remove heavy metals from solutions. This paper presents the result of studies carried out on sorption of Zn^{+2} ions from aqueous solutions by waste tea (*Camellia cinencis*) and coconut husk (*Cocos nucifera*) powder as a low cost sorbent. The biosorption experiments were performed under various conditions such as different initial metal concentrations, pH and reaction time. Characterization of the adsorbent surfaces was made after chemical modification, by using Scanning Electron Microscope (SEM), Furrier Transform Infra-Red Spectroscopy (FTIR) and 'Boehm titration' method. The optimum pH was found to be 6 for both adsorbents and different concentrations of zinc solution reached equilibrium at different ranges. About 0.25 g of modified tea waste was found to be enough to remove 38.76 mg/g of 50 g/L zinc ion concentration from 25ml metal solution and 7.9 mg/g by raw tea waste. Similarly, about 0.25 g of modified coconut husk was sufficient to remove 39.6 mg/g of 25 g/l zinc ion and 10.04 mg/g by raw coconut husk. The optimum pH was found to be 6, both the reactions followed second order kinetics and the experimental adsorption data were well fitted in both the Langmuir and Freundlich adsorption isotherm but were reasonably fitted better with the Langmuir adsorption isotherm model as compared to Freundlich adsorption isotherm model.

Keywords: Biosorption, Chemical Modification, Langmuir Isotherm, Freundlich Isotherm, FTIR, SEM

[P25] Synthesis and characterization of nanocrystalline zinc selenide

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Semiconductor nanoparticles have been a subject of interest in recent times owing to their unique and valuable photo-physical and photo-chemical properties. All these properties are dependent on crystal structure and particle size. Zinc selenide (ZnSe), a II-VI chalcogenide semiconductor, encounters extensive applications in optoelectronic devices such as photo-electrochemical cells, photoconductors, thin-film transistors, large screen LCD, LEDs, solar cells, etc. Ascorbic acid capped ZnSe semiconductor nanoparticles were synthesized by chemical precipitation method at typical room temperature at a pH of 11 using 0.1M ammonia solution. Influence of source compound of zinc and that of concentration on the size and structure of the capped ZnSe nanoparticles were studied. The sphalerite crystalline structure is settled using XRD data and SAED pattern. The average particle sizes were determined from XRD data with the help of Debye – Scherrer equation using Lorentzian profile fitting in the range of 4 nm which were further verified from TEM images.

Keywords: ZnSe Semiconductor NPs, Chemical Precipitation Method, X-ray Diffraction (XRD), Selected Area Electron Diffraction (SAED), Transmission Electron Microscopy (TEM)

[P26] Dynamics of Water Molecules Binding to Magnesium or Sodium Ions

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In biological systems, the metal caions are essential factors for activating enzymes and folding process of nucleic acids. Especially, the magnesium (Mg^{2+}) ion is one of the most ubiquitous metal ions and necessary for RNA folding and stability as well as many enzymatic reactions such as formation of complexes with ATP or GTP and transfer of phosphate groups. In order to investigate dynamics of the binding of water molecules with magnesium (Mg^{2+}), calcium (Ca^{2+}), and sodium (Na^{+}) ions, molecular dynamics (MD) simulations of those ions in aqueous solution were performed using biomolecular force fields, such as CHARMM27, AMBER03, GROMOS87, and GROMOS96 with two different water models (TIP3P and SPC). The Lennard-Jones parameters of Mg^{2+}, Ca^{2+}, and Na^{+} ions which are implemented in GROMACS 4.5.4 were used for the simulations. The resulting trajectories were analyzed in terms of structural property, time scales of binding, and dynamic behavior of water with ions, separately.

[P27] Curvature Asymmetry in Water Coalescence

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Curvature of a curved surface is an important element of fundamental phenomena in physics, chemistry, and engineering. In particular, the driving force in hydrodynamics of liquids originates from curvature and surface tension. Here we study on water coalescence of different-sized drops with curvature asymmetry through direct observations using high-resolution high-penetration ultrafast X-ray microscopy and numerical simulations. Our main result shows that curvature asymmetry between drops would play an important role in coalescence dynamics, which is unexpected in traditional theories and observations. This result helps fundamental understanding of symmetry breaking in curvature on hydrodynamics, which is applied to every fluid, not limited to water, in diverse fields.

[P28] Self-propelled motion of reactive droplets

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Wetting dynamics of a droplet on the substrate is quite different from that of pure liquid droplets by action of surfactant. The adsorption of surfactant molecules at interfaces changes wettability of the substrate, which may cause a unpredictive self-propelled motion of the droplet. Here, we show an example of that addition of Aerosol-OT (AOT) as an electrolyte surfactant into decahydronapthalene (decalin) solvent drives a droplet to move around spontaneously on a glass substrate. This phenomena is attributed to ununiform coating of AOT on the substrate surface, which would cause random temporal gradient in surface energy. Such an instantaneous surface energy gradient between coated and uncoated surfaces enables the droplet to move in random directions. We estimate the liquid-solid surface energy by measuring contact angles and surface tensions of droplets with different concetrations of AOT. The estimated value shows good agreement with our prediction. This result gives us a hint for controlling self-motion of droplets and a possibility for many potential applications relevant to microfluidics, microfabrication, and coatings.

[P29] Slowly drying of dense coffee droplets

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Coffee is a complex fluid of coffee particles that contain a thousand of chemicals. Coffee is famous as the coffee-ring effect: when a coffee drop dries on a solid surface, coffee particles move to deposit at contact lines. Using this phenomenon, evaporative lithography is under development for applications to printed electronics with patterning of soft materials such as colloids, polymers, or biomolecules. Prediction of evaporation kinetics of a complex fluid is essential to improve evaporative lithography because evaporation kinetics determines deposit patterns. Here we demonstrate experimental results that coffee drops tend to evaporate slowly as they become dense and their evaporation rates decrease linearly as ring withs grow with time. To understand the unique behavior from dense coffee drops, we propose a plausible physical mechanism based on dynamic competition between coffee-ring and porous-media flows.

[P30] Measuring mechanical properties of live cells and artificial lipid vesicles reinforced by ECM network

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In addition to regulating many phenomenon of cells, extracellular matrix(ECM) has important role in providing physical support for cells. Especially, the physical properties of cells determine stiffness of tissue and increased stiffness induced tumorigenesis in organism. However, the relationship between compositions of ECM and stiffness of individual cells is not fully understood. In this study, we investigated that the ECM compositions correlated with elasticity of cells. Micropipette aspiration provided the method for measuring physical properties of membrane of various cells and vesicles such as elasticity.

[P31] Formation of ECM-binding liposome; ECM Cellular Delivery

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We made giant unilamellar vesicles(GUVs) by electroformation. Then we attached FN or Col to the edge of the vesicles. Also we checked cell growth with different conditions of substrate for cells, Hela cells and HEK 293 cells. Fibronectin(FN) and collagen(Col) are adhesive extracellular matrix(ECM) proteins that act a crucial role in wound healing. Both proteins directly repair by regulating the behaviour of a variety of cell types that are mobilized to the damaged area in order to rebuild the tissue. However, the treatments with FN and Col are limited to wounds of the skin surface. We are currently investigating FN and Col delivery system based on liposomes which is a spherical vesicle having at least one lipid bilayer.

[P32] Gelation-induced crack prevention in colloidal films

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Crack formation is a frequent result of residual stress release from colloidal film taken by evaporation of colloidal droplets including nanoparticle. Colloidal films are widely used and have important part of industry; however, cracking in drying colloidal films can cause critical problems in application. Crack prevention is a significant task in various industries such as painting and inkjet printing with colloidal particles. Here, we suggest a versatile method to control colloid-polymer interactions by mixing a nonabsorbing polymer with a colloidal suspension, which is known to drive gelation of particles with short-range attraction. We show how colloidal drops evaporate and how cracks generate during evaporation.

[P33] Revisiting the fundamental origin of aromatic interaction

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The hydrophobic effect, the immiscible tendency for water and oil, has been readily observed in various fields and is related to quite complex components. The question of what governs the folding macromolecules towards the appropriate conformation is of great significance in many studies, especially, theoretical chemistry, molecular biology, polymer physics, pharmaceutical industry, and so on. However, it has still remained controversial and some of researchers hold a skeptical view on hydrophobic effects *per se*. While the "hydrophobicity" is a phenomenological term, the "solvation energy" is rather one of the well-defined physical quantities and readily calculated as the difference between Gibbs energies in solution and gas-phase for an ion or a molecule. We studied for the hydrophobic effects on benzene dimers. With the aid of our home-made method, a hybrid explicit/implicit solvation methodology to compute the solvation energies given by general solute-solvent pairs, we delved into the aromatic-aromatic interaction to be changed in aqueous solutions for the sandwich and T-shaped configuration of benzene dimers. In order to calculate the solvation energies, the explicit solvation method computed from the classical molecular dynamics (MD) simulation is combined with the density functional theory (DFT) calculations. The barrier energies can be observed in the binding energy curve of benzene dimers and can quantify the balance of entropy-enthalpy compensation. We expect that this study could shed light on the understanding the hydrophobic effects on various kinds of systems.

[P34] Recapitulation of Cell Surface Glycan Presentations using Multivalent Glycomaterials for Study of Influenza A Virus Specificity

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Assessing an Influenza A virus (IAV) strain for its potential risk to human health commonly begins by identifying the virus's receptor specificity towards various sialic acid (Neu5Ac) terminated cell surface glycans. Although the advent of glycan microarray technology has allowed for a detailed understanding of IAV receptor specificity switches with respect to sialic acid linkages (α2-3/α2-6), the effect of host glycan presentation on IAV recognition events remains poorly understood. Here in, we present multivalent glycopolymers displaying sialoglycans in a microarray format that we believe better recapitulates native IAV receptor binding events. In addition, this approach facilitates the collection of quantitative whole-virus binding information, which can be used to assess viral binding preference patterns across varying glycan densities and valencies in addition to polymer length. Furthermore, the flexible synthesis of the glycopolymers allows their use in multiple analytic platforms to further broaden the information that can be collected with regard to the virus and its multivalent interaction with cell surface glycans.

[P35] Single molecule Raman scattering spectroscopy under high pressure

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Vibrational blueshifts are frequently observed in high pressure Raman scattering studies. For molecular materials, such shifts reflect local compressibility as well as the strength of the anharmoic coupling between molecular vibrations and the environment. Previously reported pressure-induced blueshifts were averaged values over many molecules. Here we present a study of single-molecule Raman spectra at high pressure (1–4 GPa) in a diamond-anvil cell (DAC), with the intent of resolving different pressure-induced vibrational blueshifts of individual molecules. The molecules were two isotopologues of the dye rhodamine 6G (R6G and d4-R6G), adsorbed on colloidal Ag particles immobilized in poly(vinyl alcohol) (PVA). Single-molecule surface-enhanced Raman scattering (SMSERS) measurements were made in a confocal Raman microscope, and compared to ensemble surface-enhanced Raman scattering (SERS) measurements made in a Raman spectrometer. Spectra of mixed isotopologues in the 610 cm^{-1} region (the "isotope-sensitive" transition) allowed us to identify when the majority of spectra came from single-isotope sites, and were thereby statistically likely to arise from single molecules. There was a dramatic drop in SERS intensity when samples were pressurized in the DAC. SMSERS measurements revealed the intensity drop was caused by a pressure-induced destruction of SMSERS-active hot spots. The disappearance of hot spots was attributed to deoptimization of the gap junctions between Ag nanoparticles due to pressure-induced strain. Because the isotope-sensitive transition had little pressure-induced blueshift (<5 cm^{-1} between 0 and 6 GPa), we studied the blueshifts of a transition near 1650 cm^{-1} (the "pressure-sensitive" transition). Based on ensemble SERS measurements, this transition had a >30 cm^{-1} blueshift and a steadily increasing line width of 2.4 cm^{-1}/GPa from 0 to 6 GPa. The SMSERS spectra of this transition did not broaden as pressure was increased to 4.1 GPa. However, the variation in the blueshift of different molecules, which is characterized by the fwhm of the distribution of the measured center frequencies, increased with pressure (2.1cm^{-1}/GPa). The blueshift variation was able to account for most of the observed pressure-induced spectral broadening in an ensemble measurement. Thus the pressure-induced broadening of this R6G vibrational transition is due to the different blueshifts of different molecules.

[P36] Microrheology of semi-dilute aqueous solutions of polyethylene oxide probed by an optically trapped micro-bead

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We investigate local viscoelastic properties of semi-dilute polyethylene oxide (PEO) solutions using optically trapped polystyrene (PS) beads. In this study, we measure the motion of a micron-sized bead caused by an oscillating force produced with an optical tweezer to determine the viscoelastic moduli of the polymer solutions. To accomplish this, we use a lock-in amplifier to measure the amplitude of the particle motion and the phase difference between the movements of the particle and the tweezers as a function of the oscillation frequency. We use this approach to determine the spring constant for optical tweezers in a liquid (water) with known viscosity. We then use the spring constant to determine the frequency dependent viscoelastic moduli of polymer solutions at different concentrations. We compare results using the oscillatory optical tweezers approach (the active microrheology) with that obtained by the use of Brownian motion of the probe particle and the fluctuation-dissipation relation (the passive microrheology) in semi-dilute polymer solutions.

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