**Research**

**Protein Aggregation and Neuro-degenerative Diseases**

Our focus has been on uncovering key factors that govern protein self-assembly. We have shown that the beta structure and the population of the so-called fibril-prone conformation in the monomeric state are related to the rate of fibril formation. Based on the amyloid cascade hypothesis, the aggregation of full-length and truncated amyloid beta (Aβ) peptides is investigated to understand the molecular mechanism of Alzheimer's disease. The structural properties of the monomer and oligomers of alpha-synuclein are being studied in connection with Parkinson's disease.

**Protein Folding and Aggregation on the Ribosome**

Ribosome is a molecular machine for protein synthesis which consists of four phases of translation - initiation, elongation, termination and ribosome recycling. This process is an area of intense research due to the essential role of proteins to life. For many decades, protein folding research has been dominated by the assumption that thermodynamics determines protein structure and function. However, recently accumulated evidence has supported the emerging paradigm of non-equilibrium control of protein behavior. Namely, speed of synthesis of proteins in the ribosome greatly influences their properties, mRNA sequence evolution, and protein aggregation in bulk related to diseases. One of the main goals is explore how changes in codon translation rates affect the protein oligomerization and aggregation in bulk.

**Computer-aided Drug Design**

Combining virtual screening with molecular dynamics simulations, we search for potential drugs from large databases for a variety of diseases, including Alzheimer’s disease, cancer and Covid-19. Our predictions are further verified by our collaborators from Slovakia, Taiwan and Poland using *in vitro* and *in vivo* experiments

**Interactions of Proteins with Membranes**

Experimental studies observed that amyloid beta (Aβ) oligomers are the main pathogenic structures including effects on cognition inhibition, tau hyperphosphorylation and cellular membrane permeabilization. Oligomers can form pore in the membrane which can allow metal ions to pass through a membrane leading to neurotoxicity. In addition, these channels can cause disrupted cellular homeostasis, induce reactive oxygen species production, alter signaling pathways, and mitochondrial dysfunction. These results indicate that the molecular interaction nature between Aβ oligomers and membrane is the intriguing object to shed light on the mechanism of Alzheimer’s disease. We hypothesize that, since Aβ oligomers are more toxic than mature fibrils, they should affect membranes to a greater extent than the latter. We use MD simulations to check this hypothesis. In addition, we study the effect of metal ions such as Cu2+ and Ca2+ on the Aβ-membrane interactions.

**Methods development and applications**

We focus on development of both coarse-grained and all-atom models, which combined together to provide better results with reasonable computational cost. Our lattice models, for example, are helpful in predicting general properties of protein aggregation with and without crowders and confinement.

**Update the following materials:**

**Co-organized Events**

1. **The 5th Workshop of Vietnamese Students in Poland**

Date & place November 18-19, 2020, Warsaw, Poland

Co-chairman Mai Suan Li

More Info Conference WebPage

(http://info.ifpan.edu.pl/~masli/events/5thVietnamesestudentInPoland/index.html)

1. **The 4th Workshop of Vietnamese Students in Poland**

Date & place December 7-8, 2019, Warsaw, Poland

Co-chairman Mai Suan Li

More Info Conference WebPage

(https://www.mimuw.edu.pl/~vps/4thvsp/en/4thvsp/home.html)

1. **The 4th International Conference on Computational Science and Engineering (ICCSE-4)**

Date & place July 24 - 27, 2019, Ho Chi Minh city, Vietnam

Chairman Mai Suan Li

More Info Conference WebPage (http://conference.icst.org.vn/)

1. **Computational Biophysics at the Molecular and Mesoscales**

Date & place October 27 - 31, 2018, Quy Nhon, Vietnam

Co-chairman Mai Suan Li

More Info Conference WebPage (<https://rencontresduvietnam.org/conferences/2018/computational_biophysics/>)

1. **The First ICST Workshop on Computational Biophysics and Medicine**

Date & place October 25, 2018, Ho Chi Minh city, Vietnam

Chairman Mai Suan Li

More Info Conference WebPage

(<https://icst.org.vn/vi/news/detail/the-first-icst-workshop-on-computational-biophysics-and-medicine-278>)

1. **The 3rd Workshop of Vietnamese Students in Poland**

Date & place September 6-7, 2018, Warsaw, Poland

Co-chairman Mai Suan Li

More Info Conference WebPage

(http://info.ifpan.edu.pl/~masli/events/3rdVietnameseStudentInPoland/index.html)

1. **The 2nd Workshop of Vietnamese Students in Poland**

Date & place September 23-24, 2017, Warsaw, Poland

Co-chairman Mai Suan Li

More Info Conference WebPage

(http://info.ifpan.edu.pl/~masli/events/2ndVietnameseStudentInPoland/index.html)

1. **The 1st Workshop of Vietnamese Students in Poland**

Date & place September 24-25, 2016, Krakow, Poland

Chairman Mai Suan Li

More Info Conference WebPage

(http://info.ifpan.edu.pl/~masli/events/VietnameseStudentInPoland/index.html)

1. **The First International Conference on Computational Science and Technology (ICCST 2014)**

Date & place May 15-16, 2014, Warsaw, Poland

Co-chairman Mai Suan Li

More Info Conference WebPage

(Em tìm lại trên trang cũ của thầy)

1. **Protein Day at ICST**

Date & place December 16, 2010, Ho Chi Minh city, Vietnam

Chairman Mai Suan Li

More Info Conference WebPage

(http://info.ifpan.edu.pl/~masli/Publications/poster\_protein.pdf)

**Supervisor**

Supervised 4 PhD students. Currently supervising 7.

**Editorial work**

1. BioMed Research International, Member of the Editorial Board, section Biophysics

2.Chemical Papers, Springer, Member of the Editorial Board