



## CONFERENCE INFORMATION

### May 10, 2006, Wednesday

#### **Arrival and Registration**

Time: 9:00—10:00

Registration: Shanghai Institute for Advanced Studies (SIAS), 319 Yue Yang Road

#### **Welcome Dinner:**

Time: 18:00—19:00

Buffet: 3<sup>rd</sup> Floor, Hope Hotel, 500 Zhao Jia Bang Road

#### **Welcome Party:**

Time: 19:30—21:30

Party: Room 315, CAS-MPG Partner Institute for Computational Biology

### May 10—17, 2006

#### **Conference Lunch:**

Lunch: Shanghai Institute for Advanced Studies (SIAS), 319 Yue Yang Road

### May 13, 2006, Saturday

#### **Poster Session**

Time: 18:30-20:00

Venue: Lobby of the Students Tower

### May 14, 2006, Sunday

#### **Conference Tour: Shanghai Museum**

Time: 14:00-17:00

Meeting Place: Shanghai Institute for Advanced Studies (SIAS), 319 Yue Yang Road

### May 16, 2006, Tuesday

#### **Conference Tour: Jin Mao Tower**

Time: 17:00-20:00

Meeting Place: Shanghai Institute for Advanced Studies (SIAS), 319 Yue Yang Road

**Lecture time:** Each speaker has 90 minutes for talk and discussion.

**Conference language:** English

# PRELIMINARY PROGRAM

**Classroom:** (L) Shanghai Institute for Advanced Studies (SIAS), 319 Yue Yang Road

(P) Computer Lab of Students Tower (Open from 14:00—17:00)

(EL) Evening Lecture, Room 300, PICB, 320 Yue Yang Road



## May 10, 2006, Wednesday

Time	Speaker	Title
9:00—10:00		Arrival and Registration
10:00—11:00	Andreas Dress Frauke Gräter	<b>Welcome and Introduction, A short historical retrospect of protein dynamics and folding</b>
11:00—11:30		Coffee Break ☘ & ☕
11:30—13:00	Jane Clarke	<b>(L) Introduction: Experimentally assessing protein folding</b>
13:00—14:00		Lunch
14:00—15:30	Jane Clarke	<b>(L) More on experiments for protein folding</b>
15:30—16:00		Coffee Break ☘ & ☕
16:00—17:30	Michele Vendrusculo	<b>(L) Folding transition state</b>
18:00—20:00		Welcome Dinner
20:00—21:30		Welcome Party



## May 11, 2006, Thursday

Time	Speaker	Title
9:00—10:30	Hue Sun Chan	<b>(L) Protein folding barriers and cooperativity principles</b>
10:30—11:00		Coffee Break ☘ & ☕
11:00—12:30	Amadeo Caflisch	<b>(L) Free energies of folding and aggregation in implicit solvent</b>
12:30—13:30		Lunch
13:30—15:00	Michele Vendrusculo	<b>(L) Other non-native protein states</b>
15:00—18:00	Michele Vendrusculo	<b>(P) Folding transition state</b>
18:00—19:30		Dinner Time
19:30—21:00	Haiyan Liu	<b>(EL) Folding transition state ensembles from distributed computing</b>



## May 12, 2006, Friday

Time	Speaker	Title
9:00—10:30	Vijay Pande	<b>(L) Prediction of protein folding kinetics and energetics</b>
10:30—11:00	Coffee Break  & 	
11:00—12:30	Frauke Gräter	<b>(L) Free energies from simulations of enforced processes</b>
12:30—13:30	Lunch	
14:00—17:00	Amadeo Caflisch	<b>(P) Free energies of folding and aggregation in implicit solvent</b>
17:30—19:30	Dinner Time	
19:30—21:00	Vijay Pande	<b>(EL) Distributed computing</b>



## May 13, 2006, Saturday

Time	Speaker	Title
9:00—10:30	Michael Nilges	<b>(L) Protein structural ensembles from NMR</b>
10:30—11:00	Coffee Break  & 	
11:00—12:30	Hualiang Jiang	<b>(L) Protein-protein interactions and related drug design</b>
12:30—13:30	Lunch	
14:00—17:00	Michael Nilges	<b>(P) Protein structural ensembles from NMR</b>
17:00—18:00	Dinner Time	
18:30—20:00	Poster Session	



## May 14, 2006, Sunday

Time	Speaker	Title
9:00—10:30	William Atchley	<b>(L) Structural proteomics: from sequence to structure</b>
10:30—11:00	Coffee Break  & 	
11:00—12:30	Andreas Dress	<b>(L) Molecular evolution as a topic in mathematics</b>
12:30—13:30	Lunch	
14:00—17:30	Conference Tour: Shanghai Museum	



## May 15, 2006, Monday

Time	Speaker	Title
9:00—10:30	Rama Ranganathan	<b>(L) Coevolved sequences</b>
10:30—11:00	Coffee Break  & 	
11:00—12:30	William Atchley	<b>(L) Structural proteomics: sequence covariance</b>
12:30—13:30	Lunch	
14:00—17:00	William Atchley	<b>(P) Structural proteomics</b>
17:30—19:30	Dinner Time	
19:30—21:00	<i>Rama Ranganathan</i>	<i><b>(EL) Designing protein folds from coevolution data</b></i>

## May 16, 2006, Tuesday

Time	Speaker	Title
9:00—10:30	Helmut Grubmüller	<b>(L) Force-probe molecular dynamics: concepts</b>
10:30—11:00	Coffee Break  & 	
11:00—12:30	Hue Sun Chan	<b>(L) Desolvation and enthalpic barriers on funnel-like protein folding free energy landscapes</b>
12:30—13:30	Lunch	
14:00—17:00	Jane Clarke	<b>(P) Analyzing protein folding experiments</b>
17:00—20:00	Conference Tour: Jin Mao Tower	

## May 17, 2006, Wednesday

Time	Speaker	Title
9:00—10:30	Helmut Grubmüller	<b>(L) Force-probe molecular dynamics: applications</b>
10:30—11:00	Coffee and Closing  & 	
11:30—12:30	Lunch	