

# Viruses and Cells – Computational Challenges and Approaches

6. – 7. October 2017

Heidelberg University, Germany



UNIVERSITÄT  
HEIDELBERG  
ZUKUNFT  
SEIT 1386

Jointly with



NATIONAL YANG-MING  
UNIVERSITY

Visualization of the mechanistic details of cellular functions especially when affected by viral invasion is a keystone for improvements in nanomedicine. Computer simulations emerge as a valuable tool to supporting the endeavor.

The workshop aims to stimulate computational investigations on all scales based on biological relevant questions addressed by experimentalists. Topics will range from quantum mechanical calculations to multi scale simulations.

# Schedule:

## 6<sup>th</sup> of October 2017

9:00	Welcome	Prorektor Prof. Dieter Heermann, Heidelberg University, D Wolfgang Fischer, Biophotonics, National Yang-Ming University, Taipei, TW
9:15 – 9:40		Eric Freed, NIH, USA <i>New Insights into HIV-1 Assembly, Env Glycoprotein Incorporation, and Virus Maturation.</i>
9:40 – 10:05		Kashif Sadiq/Rebecca Wade, HITS and ZMBH, Heidelberg, D <i>Towards multiscale spatiotemporal modelling of retroviral maturation</i>
10:05 – 10:30		Frauke Gräter <i>One day in the stressful life of proteins and lipids in a tensed cell.</i>
10:30 – 11:00	Coffee Break	
11:00– 11:25		Frederik Graw, Heidelberg, D <i>Infection in space – quantifying viral transmission dynamics dependent on the tissue structure.</i>
11:25 – 11:50		Ralf Bartenschlager, Heidelberg, D <i>On the construction and deconstruction of membranous viral replication factories.</i>
11:50 – 12:15		Ulrich Schwarz, Heidelberg, D <i>The flat-to-curved transition during clathrin-mediated endocytosis: experiments and models.</i>
12:15 – 12:40		Wolfgang Fischer, NYMU, TW <i>Along a virtual cell-inspired assembly line.</i>
12:40 – 13:45	Lunch Break	
13:45 – 14:10		Jung-Hsin Lin, Taipei, TW <i>Recent Development of Methyltransferase Inhibitors against Dengue Virus with Structure- and Dynamics-Based Computational Drug Design</i>
14:10 – 14:35		Martin Ulmschneider, London, UK <i>Spontaneous assembly of functional membrane channels from soluble membrane active peptides.</i>
14:35 – 15:00		Martin Zacharias, TU München, D <i>Investigating peptide-protein binding and antigen presentation using docking and MD simulations.</i>

15:00 – 15:30	Coffee Break
15:30 – 15:55	T. Cross, Tallahassee, FL, US; <i>Solid State NMR and Computations the Tricky Path to Functional Understanding in Membrane Proteins.</i>
15:55 – 16:20	Yueh-Hsin Ping, Taipei, TW <i>Virus-host interactions - Lessons learned from single-virus tracking.</i>
16:20 – 16:45	Andrew J. Spakowitz, Stanford, CA, USA <i>Modeling the Physical Processes Underlying Epigenetic Regulation.</i>
16:45 – 17:00	Closing Remarks for the day
19:30	Dinner

## 7<sup>th</sup> of October 2017

9:15 – 9:40	Klaus Strebel, Bethesda, MD, USA <i>Identification of a novel tetherin-like restriction of HIV particle release in macrophages.</i>
9:40 – 10:05	Mark Sansom, Oxford, UK <i>Molecular Simulations to Characterise Cell and Viral Membranes and Their Interactions.</i>
10:05 – 10:30	Paolo Carloni, Jülich, D <i>Multi-scale simulations of G-protein coupled receptors.</i>
10:30 – 10:45	Coffee Break
10:45 – 11:10	Rainer Böckmann, Erlangen, D <i>Peptide-Lipid Interaction.</i>
11:10 – 11:35	Urs Greber, Zurich <i>Principles of Virus Entry &amp; Egress by Wet-Lab &amp; Computational Approaches.</i>
11:35 – 12:00	Rainer Fink, Heidelberg, D <i>Quantification of Ca-Regulation in Mikrodomains of Muscle as Viral Targets.</i>
12:00 – 12:10	Closing Remarks
12:10 – 13:30	Lunch