## 7<sup>th</sup> Ringberg Workshop on Structural Biology (with XFELs)

|         |                   | Wednesday, February 14 <sup>th</sup> , 2024  |
|---------|-------------------|--|
| > 15:00 |                   | Coffee, cake, Garden room  |
|         |                   | Chair: Richard Bean  |
| 16:20   | Ilme Schlichting  | Welcome  |
| 16:30   | John Beale        | Fun and games with fixed-targets at SwissFEL's Cristallina experimental station  |
| 17:00   | Sebastian Günther | Room temperature X-ray fragment screening with serial crystallography  |
| 17:30   | Frédéric Poitevin | The data reduction challenge for LCLS-II imaging experiments - current and future strategies for end-to-end online analysis                        |
| 18:00   | Lois Pollack      | Watching RNA fold: a new approach to time-resolved solution scattering at XFELs  |
| 18:30   |                   | Dinner   |
|         |                   |  |
|         |                   |  |
|         |                   | Thursday, February 15th, 2024  |
|         |                   | Chair: Jaehyun Park  |
| 9:00    | Rick Kirian       | Nanojet Fluctuation X-Ray Scattering   |
| 9:30    | Kartik Ayyer      | Single particle X-ray imaging: The road to sub-nm resolution   |
| 10:00   | Helmut Grubmüller | De novo structural ensemble determination from single-molecule X-ray scattering: A Bayesian approach   |
| 10:30   |                   | Coffee break   |
|         |                   | Chair: Eriko Nango   |
| 11:00   | Philip Johnson    | Ultrafast optical excitation of photoactive proteins   |
| 11:30   | Thomas Barends    | Influence of Illumination Conditions on Myoglobin in TR-SFX-experiments  |
| 12:00   | John Kennis       | Facile two-photon absorption and photoionization of a bacterial phytochrome: implications for time-resolved X-ray crystallography and spectroscopy |

| 12:30<br>12:40 |                     | Group photo (depending on weather) Lunch   |
|----------------|---------------------|--|
| 12.40          |                     | Chair: Jennifer Wierman  |
| 14:00          | Emina Stojković     | Capturing bacterial phytochrome in action  |
| 14:30          | TJ Lane             | Time-resolved crystallography captures light-driven DNA repair   |
| 15:00          | Dominique Bourgeois | Conformational heterogeneity in phototransformable fluorescent proteins viewed by NMR, optical spectroscopy and crystallography. |
| 15:30          |                     | Coffee break   |
|                |                     | Chair: Nanna List  |
| 16:00          | Helen Ginn          | Teasing out the secrets of subtle protein dynamics   |
| 16:30          | James Holton        | Untangling models for less noisy maps  |
| 17:00          | Derek Mendez        | Deep residual networks for crystallography trained on synthetic data   |
| 17:30          | Frank Noé           | What can Generative AI do for structural biology?  |
| 18:00          |                     | Tour of the castle   |
| 18:45          |                     | Dinner   |
|                |                     | Chair: Miquel Huix-Rotllant  |
| 20:00          | Mark Wilson         | Open Questions about Quantum Mechanical Charge Transfer in Proteins  |
|                | Alice Walker        | Large-scale quantum mechanics simulations of extended electronic effects in ICH Ralstonia  |
|                |                     |  |
|                |                     |  |
|                |                     | Friday, February 16th, 2024  |
|                |                     | Chair: Karin Kühnel  |
| 9:00           | Radoslav Enchev     | Time-resolved cryo-EM: methods development and applications  |
| 9:30           | Ulrich Lorenz       | Microsecond time-resolved cryo-EM  |
| 10:00          | Holger Stark        | Breaking the ice: CryoEM's quest for better resolution and quality   |

| 10:30 | Coffee break |
|-------|--------------|
|       |              |

|              |                             | Chair: Adi Natan   |  |
|--------------|-----------------------------|--|--|
| 11:00        | Henry Chapman               | Opportunities for imaging at high temporal and spatial resolution  |  |
| 11:30        | Andrew Aquila               | X-ray Quantum Imaging  |  |
| 12:00        | Doeke Hekstra               | Mapping the reaction coordinates of proteins by X-ray crystallography  |  |
| 12:30        |                             | Lunch  |  |
| 14:00        | Discussion rounds / Hiking  |  |  |
| 18:30        |                             | Conference Dinner  |  |
|              |                             | Chair: Marco Cammarata   |  |
| 20:30        | Philip Anfinrud             | What can we learn from temperature-dependent, time-resolved SAXS/WAXS studies of biomolecules using synchrotron radiation? |  |
|              |                             | Saturday, February 17th, 2024  |  |
|              |                             | Chair: Allen Orville   |  |
|              |                             |  |  |
| 9:00         | Clare Megarity              | Electrical Control of Enzyme Cascades under Crowded Nanoconfinement  |  |
| 9:00<br>9:30 | Clare Megarity Stephen Carr |  |  |

Monitoring penicillin ring formation through a crystallographic and spectroscopic lens

## 11:15 End of meeting, lunch packages if desired

Patrick Rabe

10:30