

## **Session Program**

**19-22 Sept 2022**

# **Machine Learning in Natural Sciences: from Quantum Physics to Nanoscience and Structural Biology**

## **Molecular Structure Analysis**

CFEL (Building 99), Seminarraum 1-3  
Luruper Chaussee 149 22761 Hamburg Germany

# Wednesday 21 September

09:00

## Molecular Structure Analysis

**Session** | **Location:** CFEL (Building 99), Seminarraum 1-3, Luruper Chaussee 149 22761 Hamburg Germany

09:00–09:45

### AI Usage in Structural Biology

**Speaker**

Dr Andrea Thorn

09:45–10:00

### Chiral Structure Classification by a Convolutional Neural Network

**Speaker**

Peer Kasten

10:00–10:15

### Learning Conductance: Gaussian Process Regression for Molecular Electronics

**Speaker**

Michael Deffner

10:30

11:00

## Molecular Structure Analysis

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11:00–11:45

### OpenFold: Democratizing access to modeling biomolecules and their interactions

**Speaker**

Prof. Mohammed AlQuraishi

11:45–12:15

### Quantum flows neural network for variational solutions of the Schrödinger equation

**Speaker**

Andrey Yachmenev

12:30