



Contribution ID: 16

Type: **Talk**

## Deciphering protein conformational dynamics with cryo-EM and MD simulations

*Tuesday, 13 February 2024 15:00 (25 minutes)*

Cryo-Electron Microscopy (cryo-EM) allows conformational studies of macromolecular complexes in their close-to-native state, essential for understanding their working mechanisms and for structure-based drug development. However, deciphering continuous conformational transitions of macromolecules, through the main cryo-EM processing techniques, Single Particle Analysis (SPA) and cryo-Electron Tomography (cryo-ET), is challenging partly due to the low signal-to-noise ratio. I will present new image processing methods based on Molecular Dynamics (MD) simulations that allow extracting continuous conformational variability from SPA and cryo-ET data.

### Submitting to:

Integrative Computational Biology workshop

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**Session Classification:** Protein conformational flexibility and solution experiments