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# Conference on Frontiers in Atomistic Simulations: from Physics to Chemistry and Biology | (smr 4098)

Tuesday 09 September 2025

**notitle - Budinich Lecture Hall (LB) (14:00-18:10)**

***Chair: Francesco Gervasio (University of Geneva)***

time	title	presenter
14:00	Integrative structural biology in the era of Artificial Intelligence	MAX BONOMI
14:30	Brain injury and cancer, two sides of the same coin?	SIMONA PARRINELLO
15:00	Making sense of biomolecular trajectories in the exascale era	JAYASHRITA DEBNATH
15:30	Coffee break	
16:10	TBA	CRISTOPH DELLAGO
16:40	From Stability to Dissociation: Elucidating Unbinding Kinetics of Protein-Protein Complexes via Atomistic Simulations	OMAR VALSSON
17:10	Have you tried turning it off and on again? Stochastic resetting for enhanced sampling	BARAK HIRSHBERG
17:40	Electronic stopping in liquid water, vapor, ice, and DNA from TDDFT	JORGE KOHANOFF