#	Last Name, First Name	Oral Title on-site
16	Hummer, Gerhard	Towards Cell-Scale Molecular Simulations
40	<b>Anthony Raj,</b> Xavier Prasanna	Mechanistic Insight into Seipin's Activity During Initial Stages of Lipid Droplet Formation
180	Juber, Anna Selina	Thermodynamic Driving Forces of Guest Confinement in a Photoswitchable Cage
263	Kav, Batuhan	Does the Inclusion of Polarisability Lead to a Better Modelling of Peptide Aggregation?
328	Briand, Eliane	Constant pH Molecular Dynamics in GROMACS using Lambda Dynamics and the Fast Multipole Method
339	Lapierre, Jeremy	DNA Opening During Transcription Initiation by RNA Polymerase II in Atomic Detail
351	Buslaev, Pavel	Constant pH MD in GROMACS
381	Diez, Georg	Identifiying Collective Motion in Proteins - Divide and Conquer the Feature Space
414	Ives, Callum M.	A Cooperative Knock-On Mechanism Underpins Ca2+-Selective Cation Permeation in TRPV Channels
432	Faber, Christian	A New Measure for Contact Maps
441	Versini, Raphaëlle	Structural Basis of the Transmembrane Domain of the Yeast Mitofusin Fzo1
449	<b>Durumeric,</b> Aleksander	Towards Quantitatively Accurate Neural Network CG Force-fields
506	Gomez Flores, Claudia Leticia	Thiol-Disulfide Exchange Reactions Using an Artificial Neural Network Corrected DFTB/MM Methodology
509	Michelarakis, Nicholas	Avidity of the Malaria Adhesin VAR2CSA is Mechano-Controlled by Exposure of a Second Cryptic CSA Sugar Binding Site
520	König, Melanie	Membrane Curvature Induced Lipid Sorting in Coarse-Grained Simulations
526	Jung, Hendrik	Artificial Intelligence for Molecular Mechanism Discovery
527	Schäfer, Stefan	Anchoring of the SARS CoV-2 Fusion Peptide in Host Membranes
531	Sztain, Terra	Weighted Ensemble Simulations of SARS-CoV-2 Glycosylated Spike Opening
536	<b>Igaev,</b> Maxim	Bending-Torsional Elasticity and Energetics of the Plus-End Microtubule Tip

## List of Oral Contributions, Hybrid Workshop, April 08-09, 2022 2022-07-04 "COMPUTER SIMULATION AND THEORY OF MACROMOLECULES"

#	Last Name, First Name	Oral Title online
103	Mandal, Nabanita	Mechanistic Insights into the Differential Dynamics of SARS-CoV-2 Variants of Concern (VOC)
340	Çetin, Ebru	Manipulation of a Cryptic Site on DHFR to Combat Trimethoprim Resistance in E. coli
380	Lam, Chun Kei	Identification of Gating Sensitive Residues in TREK-2
486	Vossel, Maximilian	Local Mode Softening versus Hardening Underpins Specific Allosteric Responses
501	McGrath, Hugo	Peptide Deformylase as a Probe of Long-Range Allostery Through the Ribosomal Protein uL22