



# ESS-ILL user meeting - topical session on atomic-scale simulations in neutron scattering

## Thursday, 21 January 2021

### Soft matter (incl. biology) (13:00 - 15:05)

time	[id] title	presenter
13:00	[4] Enhancing refinement with quantum mechanics in neutron protein crystallography	CALDARARU, Octav
13:25	[14] New on-line DFT approach to analyse neutron diffraction crystallography and SANS data	GENOVESE , Luigi CRISTIGLIO , Viviana
13:50	[29] Diffusive-like motions in a solvent free myoglobin-polymer hybrid revealed by neutron scattering and MD simulations.	FICHOU, Yann
14:15	[25] LiquidLib: An MPI/OpenMP Parallelized Toolbox for Analyzing Molecular Dynamics Simulations with Applications to Neutron Scattering Experiments	ZHAI, Yanqin
14:40	[8] Using molecular modeling and neutron scattering experiments to investigate PNIPAM microgels	TAVAGNACCO , Letizia