



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

## Wednesday, 20 January 2021

### Nanomaterials & Liquids: 2 (16:00 - 18:30)

time	[id] title	presenter
16:00	[9] An investigation of 3He in C60: A DFT, theoretical and INS study	AOUANE , Mohamed
16:25	[10] Neutron scattering and MD simulations applied to geo-inspired nanotubes	D'ANGELO , Arianna
16:50	[26] Water dynamics in carbon nitride – a joint QENS, DFT and AIMD study.	LISOWSKA, Karolina
17:15	[31] THE STRUCTURE OF WATER IN CALCIUM-SILICATE-HYDRATES STUDIED BY NEUTRON DIFFRACTION WITH ISOTOPIC SUBSTITUTION.	Mrs ZHAKIYEVA, Zhanar
17:40	[32] Neutron reflectivity and MD simulation study of ionic liquids and deep eutectic solvents at a solid electrode	ZEC, Nebojsa