

PROGRAM OF THE WORKSHOP:

DAY 1.	
9:00-9:15	Welcome 14 th USPEX workshop – Alexander P. Kuleshov, Artem R. Oganov
9:15-10:15	Artem R. Oganov MAE “Crystal structure prediction and the USPEX code”
10:15-11:00	Alexey V. Yanilkin “Hot problems in materials science”
11:00-11:15	Tea break
11:15-12:00	Jun Li “ Dynamical single-atom catalysis with nanoparticles”
12:00-12:45	Xavier Gonze “Introduction to density functional theory”
12:45-14:30	LUNCH & posters
14:30-15:15	Vladislav A. Blatov “Topological methods in crystal chemistry”
15:15-16:00	P.V. Bushlanov “Topological generator of crystal structures”
16:00-17:00	TUTORIAL 1 : Installation party: first steps with USPEX (Artem I. Samtsevich)
17:00-19:00	TUTORIAL 2: Predicting high-pressure phases with USPEX (Artem R. Oganov)
19:00	DINNER (separately)
DAY 2.	
9:00-9:45	Alexey Lukoyanov “Correlated electrons and post-DFT methods”
9:45-10:15	Zahed Allahyari “Multiobjective optimization as a tool for materials discovery”
10:15-10:45	Alexander G. Kvashnin “Search for materials with optimal properties”
10:45-11:30	Qiang Zhu “Constrained global optimization for molecular crystals, surfaces, interfaces, polymers and nanoparticles”
11:30-11:45	Tea break and Group photo
11:45-12:30	Albert Nasibulin “Carbon nanomaterials: materials of the future”
12:30-12:45	Sergey V. Lepeshkin “Searching for magic nanoparticles with USPEX”
12:45-14:30	LUNCH & posters
14:30-16:00	<i>TUTORIAL 3: Molecular crystals (Qiang Zhu and Valery Royzen)</i>

16:00-17:00	<i>TUTORIAL 4: Variable-composition structure prediction (Artem R. Oganov)</i>
17:00-19:00	<i>TUTORIAL 5: Surfaces and nanoparticles (Oleg Feya and Artem R. Oganov)</i>
19:00	DINNER (separately)

DAY 3.

9:00-9:45	Yulia Gorbunova MAE “Materials of the future: artificial photosynthesis, artificial muscles, artificial vision”
9:45-10:30	Artem R. Oganov “New methods in the USPEX code”
10:30-11:15	Vladislav A. Blatov “Topological methods for predicting phase transition mechanisms”
10:15-11:00	Artem I. Samtsevich “Predicting phase transition mechanisms with USPEX”
11:00-11:15	Tea break
11:15-12:00	Alexander Shapeev “Machine learning potentials: expanding the power of computational materials discovery”
12:00-12:30	Sergey Pozdnyakov “Recent progress with machine learning methods”
12:30-12:45	Dmitry Semenok “Predicting novel high-temperature superconductors”
12:45-14:30	LUNCH & posters
14:30-15:00	Ivan Kruglov “Towards protein structure prediction”
15:00-16:45	<i>TUTORIAL 6: Evolutionary metadynamics (Artem R. Oganov)</i>
16:45-18:00	<i>TUTORIAL 7: Variable-cell nudged elastic band method (Artem I. Samtsevich)</i>
18:00	<i>Start moving to banquet place</i>
19:00	<i>DINNER (workshop banquet)</i>