15th workshop "Crystal structure prediction with USPEX code"
Moscow, 17-19 September, 2018
Skoltech,
Nobel street, Bld. 3
4th floor, Room 407-408

SEPTEMBER 17

9:30-10:00	*Registration of participants*
10:00-10:15	Welcome 15th USPEX workshop – **Alexander P. Kuleshov, Artem R. Oganov**
10:15-11:15	**Artem R. Oganov** "Crystal structure prediction and the USPEX code"
11:15-11:30	*Tea break*
11:30-12:15	**Andrey V. Shevelkov** "Structure-property relationships in thermoelectric clathrates"
12:15-13:00	**Xavier Gonze** "Introduction to density functional theory"
12:30-14:30	*LUNCH* & posters
14:30-14:45	**Hubert Valencia** "Integration of USPEX to GDIS visualization software"
14:45-16:30	*TUTORIAL 1*: Installation party: first steps with USPEX (**Artem I. Samtsevich**)
16:30-17:30	*TUTORIAL 2*: Predicting high-pressure phases with USPEX (**Artem R. Oganov**)
17:30-18:00	*DINNER (separately)*
18:00-19:30	*TUTORIAL 3:* Molecular crystals (**Valery Royzen** and **Artem R. Oganov**)

SEPTEMBER 18

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"
10:45-11:00	*Tea Break*
11:00-12:00	*Excursion in Skoltech campus and group photo*
12:00-12:45	**Albert Nasibulin** "Carbon nanomaterials: materials of the future"
12:45-13:00	**Sergey V. Lepeshkin** "Searching for magic nanoparticles with USPEX"
13:00-14:15	LUNCH & posters
14:15-15:00	**Vladislav A. Blatov** "Topological methods in crystal chemistry"
15:00-15:45	**Pavel Bushlanov** "Topological generator of crystal structures"
15:45-16:45	*TUTORIAL 4:* Variable-composition structure prediction (**Artem R. Oganov**)
16:45-18:00	*TUTORIAL 5:* Nanoparticles (**Vladimir Baturin**)
18:00	*Start moving to banquet place*
19:00	*DINNER (workshop banquet)*

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SEPTEMBER 19	
9:30-10:30	**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*
11:15-11:30	**Alexander G. Kvashnin** "Predicting novel high-temperature superconductors"
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"
12:30-13:00	**Ivan Kruglov** "Towards protein structure prediction"
12:45-14:30	LUNCH & posters
14:30-16:15	*TUTORIAL 6:* Evolutionary metadynamics (**Artem R. Oganov**)
16:15-17:45	*TUTORIAL 7:* Variable-cell nudged elastic band method (**Artem I. Samtsevich**)
17:45-18:30	*DINNER (separately)*
17:45-18:30	*FREESTYLE (Solving participants' problems, answering questions)*