USPEX SCHOOL 2021

Workshop 17-19 November

Skoltech online

20th workshop on crystal structure prediction with USPEX code (20th Lyakhov school)

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Language: English

Program can be found here

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The workshop is organized by Prof. Artem R. Oganov and Dr. Vladimir Baturin.

Crystal structure prediction recently emerged as a powerful approach to predict new materials. The ambitious goal to replace an Edisonian trial-and-error routine by the artificial intelligence has given rise to a number of approaches. Being also a powerful instrument for discovering new phenomena at extreme conditions, crystal structure prediction should thus be an everyday tool at the hands of nearly every computational materials scientist.

The evolutionary algorithm USPEX proved to be a very efficient and reliable method, and the USPEX code, based on it and freely distributed to academic scientists, is currently used by >7600 researchers worldwide and this number grows rapidly. We should note that in addition to the evolutionary structure prediction, USPEX code features many other techniques (random sampling, metadynamics, minima hopping, particle swarm optimization) and familiarity with this code will give solid background in many structure prediction techniques. This regular series of pedagogical events brings these topics to new generation of materials scientists.

This year our traditional workshop will be held in online format. The comprehensive lectures on the theoretical foundations of materials science and reports of the bleeding edge discoveries in our field will be followed by detailed tutorials from the developers of the USPEX code.

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RSF | Russian Science Foundation
Project number 17-73-30006

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