Computational Materials Discovery Using Evolutionary Algorithm USPEX

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In the last decade, a number of approaches made it possible to discover new materials on the computer – prior to experimental verification. This holds a transformative potential for the development of new technologies. A special role in this development is played by our evolutionary algorithm USPEX, developed by me and my students since 2006. The methodology will be reviewed along with applications to several problems of materials science.

To enable discovery of technologically useful materials, we implement multiobjective (Pareto) optimization and apply it to a variety of problems: Our new method, Mendelevian Search, capable of finding the best materials among all possible compounds with all possible crystal structures, will be described and its results illustrated.

I will describe results of our recent works along several lines: 1. Search for novel thermoelectric materials, where we show the possibility of achieving the figure of merit ZT>>1. 2. Discovery of novel superhard materials. 3. Prediction of new high-temperature superconductors. 4. Prediction of novel chemistry of nanoparticles and possible explanation of carcinogenicity of oxide dust.

Current limitations and future prospects of these methods will be discussed.