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Skolkovo Institute of Science and Technology

Energy Colloquium

Computational Materials Discovery

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Skolkovo Innovation Center

Technopark, Building 3, Room 402

ABSTRACT:

Thanks to powerful evolutionary algorithms, in particular the USPEX method, it is now possible to predict both the stable compounds and their crystal structures at arbitrary conditions, given just the set of chemical elements. Recent developments include major increases of efficiency, extensions to low-dimensional systems and molecular crystals (which allowed large structures to be handled easily, e.g. $Mg(BH_4)_2$ and H_2O-H_2), machine learning for accelerated calculations, and new techniques called evolutionary metadynamics and Mendelevian search.

Some of the results that I will discuss include:

1. Theoretical and experimental evidence for a new partially ionic phase of boron, ?-B and an insulating and optically transparent form of sodium.
2. Predicted stability of "impossible" chemical compounds that become stable under pressure - e.g. Na_3Cl, $NaCl_3$, $NaCl_7$, Mg_3O_2, MgO_3, SiO, SiO_3.
3. Novel low-dimensional phases of boron (semiconducting vs metallic boron surface reconstructions, recently synthesized borophene, and predicted magnetic 2D-boron), surface reconstructions of TiO_2 and SiO_2, metal oxide nanoparticles.
4. Novel dielectric polymers, and novel permanent magnets confirmed by experiment and ready for applications.
5. Prediction of new hard and superhard materials.

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Colloquium schedule and information on how to get to the colloquium can be found at *http://www.skoltech.ru/en/energy-colloquium/*