Novel methods for predicting exotic compounds and new materials

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Until mid-2000s it was thought that crystal structures are fundamentally unpredictable. This has changed, and a special role in this transformation was played by our evolutionary method USPEX. Thus method can be viewed as a type of artificial intelligence, and routinely allows one to predict stable crystal structures for a given chemical composition], predict all stable compounds formed by given elements, and even predict among all possible compounds the structure and composition that have desired combination of properties. Here I will discuss:

1. Discovery of novel chemical phenomena at high pressure: transparent non-metallic allotrope of sodium, counterintuitive novel sodium chlorides, chemical reactivity of helium, prediction and discovery of new high-temperature superconducting polyhydrides, approaching room-temperature superconductivity.
2. Recent extension of crystal structure prediction to finite temperature, and first results for planet-forming materials.
3. Development of coevolutionary methods – COPEX (to predict all stable compounds in very complex systems) and Mendelevian search (navigating the chemical space to find the material with desired properties).

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