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Reactivity of elements and compounds:results of sructure prediction algorithmUSPEX

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Recent developments in crystal structure prediction, in particular, the powerful evolutionary algorithm USPEX [1,2], enable reliable prediction of stable compounds formed by given elements. At normal conditions such calculations produce the well-known stable compounds: e.g., NaCl as the only compound of Na and Cl, or MgO as the only stable compound of Mg and O. At high pressures and in low-dimensional materials, unexpected phenomena have been predicted – then experimentally verified. I will discuss several recent examples:

1. Discovery of two new stable high-pressure compounds of helium, Na2He and Na2HeO (Na2He has been synthesized experimentally) [3]. This discovery has implications for both fundamental chemistry and planetary sciences.
2. Formation of new stable sodium chlorides: Na3Cl, Na2Cl, Na3Cl2, NaCl3, NaCl7 [4], Na4Cl3 [5], and a large number of new stable potassium chlorides [6]. These predictions were verified experimentally [5,6] and are still not fully understood.
3. New stable magnesium oxides: Mg3O2 and MgO2 [7] and MgO3 [8], and silicon oxides SiO and SiO3 [8]. Among these predictions, stability of MgO2 has already been experimentally confirmed [9]. These predictions may have implications for planetary chemistry.
4. USPEX-based prediction of the Cui group [10] and experimental verification of Eremets group [11] of a new high-temperature superconductor – cubic H3S. This discovery opens new hopes for room-temperature superconductivity.
5. Prediction [12] that dominant silicon oxide nanoparticles at normal conditions (ambient P-T, and normal air) will be oxygen-enriched and magnetic: e.g. Si7O19. This may explain well-documented carcinogenic activity of fine silica dust.
Future avenues for explanation and generalization of these phenomena will be discussed.

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