Structure prediction and behavior of (un)known materials in extreme conditions

Dejan Zagorac[1,2], Jelena Zagorac[1,2], Tamara Škundrić[1,2], Milan Pejić[1,2], Dušica Jovanović[1,2], Klaus Doll[3], Christian J. Schön[4], Branko Matović[1,2]

[1]Institute of Nuclear Sciences "Vinča", Materials Science Laboratory, University of Belgrade, Belgrade, dzagorac@vinca.rs Serbia, [2]Center of excellence "CextremeLab", Center for synthesis, processing, and characterization of materials for application in the extreme conditions, Belgrade, Serbia, [3]Institute for Theoretical Chemistry, University of Stuttgart, Germany, [4]Max Planck Institute for Solid State Research, Nanoscale Science Department, Stuttgart, Germany.

Over the years scientists have begun research to invent materials sustainable under extreme conditions. Furthermore, such innovative materials explored at high pressures, under high magnetic and electric fields, over a wide range of temperatures, radiation conditions, corrosive environments, under extreme mechanical loads, and non-equilibrium thermodynamic conditions are applicable not only in e.g. deep ocean explorations or space travel but become increasingly relevant in our daily life, such as in applications to energy production and conversion, maintenance of the water supply, or the stability of the computer infrastructure under coronal mass ejections. In that respect, we show the results of well-known barium sulfide (BaS) compound, where novel predicted and previously synthesized BaS phases have been calculated and subjected to extreme pressures up to 100GPa. The structure-property relationship and in particular metalization of BaS has been investigated in detail [1,2]. Boron suboxide, B_6O is the third hardest material after diamond and c-BN and the hardest known oxide. Here, we present structure prediction, high-pressure effect, and properties investigation of superhard B_6O [3,4]. Finally, we present one unknown Cr_2SiN_4 compound calculated using a combination of Density-functional theory (DFT), data mining (DM), global optimization (GO), as well as the newly developed Primitive Cell approach for Atom Exchange (PCAE) method [5]. Moreover, the behavior of the predicted Cr_2SiN_4 compound under high pressure up to 10 GPa has been investigated.

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