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

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Novel predicted and previously synthesized BaS phases have been calculated and subjected to extreme pressures. The structure-property relationship and in particular metalization of BaS has been investigated. Here, we present structure prediction, high-pressure effect, and properties investigation of superhard B6O. Finally, we show one unknown Cr2SiN4 compound calculated using a combination of the theoretical methods, and behavior under high pressure has been investigated.

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