Abstract Submitted
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Study on the formation of rhenium borides by density functional calculations R.R. AGUNDEZ, Facultad de Ciencias, UABC, G. SOTO, M.G. MORENO, A. REYES-SERRATO, Centro de Nanociencias y Nanotecnologia, UNAM — The searching of hard and superhard materials is a hot topic in material science. Two known factors are fundamental to get high hardness: (1) high valence-electron density; and (2) high number of electron in covalent bonds. The 5d-transition metals comply with requirement (1); so, the task is to fulfill condition (2) without expanding its native structure. Supposedly this is possible by developing interstitial alloys with elements of moderate electronegativity, like boron and/or carbon. This idea materializes in the very hard ReB2, which scratches the surface of diamond. This work is a study in the formation of rhenium borides by density functional calculations. Here, we want to reveal the changes that would occur in the hexagonal close packed lattice of Re as B is inserted into its interstitial sites. We cover compositions in ReBx from x = 0 to x = 3 in x steps of 0.125. B is positioned in octahedral and tetrahedral interstices of Re, and for each arrangements we have calculated cell volume, cohesive energy, bulk modulus, valence electron concentration, and energy density. Supported by FONDOS CONACYT I0013, SNI-ESTUDIANTES 2008-01, SOLICITUD: 103909

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