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Stable Compound of Helium and Sodium at High Pressure

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Helium (He) is, on par with Neon, the most inert element in the Periodic Table. Indeed, no conclusive proofs about stable compounds containing chemical bonds with He at ambient conditions have been reported so far. However, pressure significantly affects chemical properties of elements. By using USPEX [1], a software which has been successfully used in the past to predict unexpected high pressure crystal structure [1], we found that above 160 GPa He and Sodium exothermically combine to form the compound Na2He, whose structure is reported in Fig. 1. Quasiharmonic free energy calculations based on computed phonon spectra indicate that the free energy of formation of Na2He is negative and that the latter is barely affected by the temperature (0-800 K range was considered). In order to understand the cause of stability of Na2He, we carried out a thorough study of its electronic structure at various pressures by means of several different approaches including the examination of the band structure and the analysis of real-space descriptors such as the electron density in the framework of the Quantum Theory of Atoms in Molecules [2], the Electron Localization Function [3] and the deformation density. By examining the band structure, we found that such compound is an insulator whose band-gap increases with pressure. Regarding real-space descriptors, two remarkable features of Na2He are the negative charge on He (obtained both using Mulliken and Bader partitioning) and the presence of interstitially localized electrons (i.e. Non-Nuclear Attractors), the latter being detectable in all the analyses above mentioned. In the range 160-350 GPa, the exothermicity associated to the formation of Na2He is mainly due to the volume reduction, while at higher pressures the electronic energy plays a prominent role in the stabilization of this compound. In this contribution we present the results of our study with particular emphasis on the role played by He in the stabilization of Na2He.

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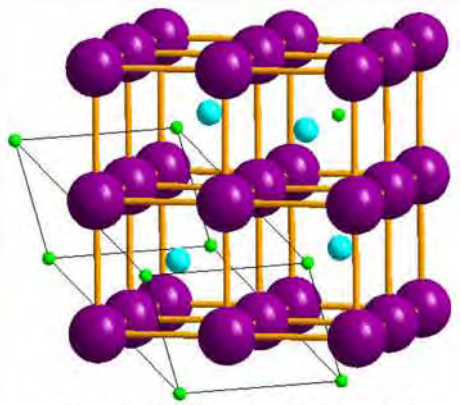

Figure 1. Crystal structure of Na_2He. Violet=Na, Blue=He, green=non-nuclear attractors. Primitive cell in solid lines

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