

Abstract

# Rubidium at Extreme Conditions †

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Transformations of alkali metals at high pressures is one of the hot topics of modern condensed matter physics. Exotic crystalline structures with very large and complex unit cells, unusual melting lines showing maxima and minima, pressure induced metal to non-metal transitions are some examples of this fascinating scenario. I will describe recent X-ray diffraction (XRD), Raman spectroscopy and Inelastic X-ray Scattering (IXS) studies on liquid and solid Rubidium at extreme pressures, up to several tens of GPa. XRD and IXS data in diamond anvil cells (DACs) consistently show a liquid–liquid transformation from a simple metallic liquid to a complex one, occurring at 6.5–8.5 GPa, which is slightly above the first maximum of the T–P melting line [1,2]. This transformation is traced back to the density-induced hybridization of highest electronic orbitals (*s-d* transition) leading to the accumulation of valence electrons between Rb atoms and to the formation of interstitial atomic shells, a behavior that Rb shares with Cs and is likely to be common to all alkali metals. Similarly, in the solid state, compressed alkali metals up to tens of GPa exhibit complex low-symmetry modifications, due to the density-driven transition of the valence electrons from the *s* state to states of higher angular momentum. We conducted challenging Raman spectroscopy measurements in DACs and *ab initio* computer simulations on the optical phonons of the low symmetry, high pressure crystalline phases of Rb up to 100 GPa [3]. The relative (relative to the normal condition value) density behavior of Raman frequencies of Rb is compared to that of Na and Li, once the frequencies of the two light alkali elements have been properly rescaled by their masses. Importantly, while the rescaled density behaviors of Na and Li agree with each other, Rb significantly differs, which highlights the different nature of the valence electron transition being of the *s-d* and of the *s-p* type in heavy and light alkali metals, respectively, a result that calls for further similar investigations of K and Cs. *Ab initio* simulations help the data analysis and show the evolution of the electronic, structural and dynamic properties in Rubidium extending to conditions still difficult to reach experimentally.

## References

1. Gorelli, F.A.; de Panfilis, S.; Bryk, T.; Ulivi, L.; Garbarino, G.; Parisiades, P.; Santoro, M. Simple-to-Complex Transformation in Liquid Rubidium. *J. Phys. Chem. Lett.* **2018**, *9*, 2909–2913.
2. Bryk, T.; De Panfilis, S.; Gorelli, F.A.; Gregoryanz, E.; Krisch, M.; Ruocco, G.; Santoro, M.; Scopigno, T.; Seitsonen, A.P. Dynamical Crossover at the Liquid-Liquid Transformation of a Compressed Molten Alkali Metal. *Phys. Rev. Lett.* **2013**, *111*, 077801, doi:10.1103/PhysRevLett.111.077801.
3. Santoro, M.; Colognesi, D.; Monserrat, B.; Gregoryanz, E.; Ulivi, L.; Gorelli, F.A. High-pressure vibrational properties of dense rubidium. *Phys. Rev. B* **2018**, *98*, 104107, doi:10.1103/PhysRevB.98.104107.



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