Joint Theory Seminar

European XFEL, CFEL & Prof. Lichtenstein's Group at University of Hamburg

Thursday, 5 May 2022, 16:00 – 17:00 via Zoom

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Materials discoveries at extreme conditions: from curiosity driven research to advanced functionalities

In collaboration between theory and experiment, we explore materials behavior at pressure up to 1 TPa. Focusing on oxides and nitrides, we present an overview of materials discovered recently at the multimegabar compressions. We demonstrate that they have fascinating crystallochemistry and physical properties challenging accepted concepts, like Pauling's rules [1] and concept of valence [2]. Considering high-pressure cubic FeO2 and complex and unusual carbonate, Fe3CO7, we show that oxygen has a formal valence less than 2. Our DFT+DMFT calculations reproduce and explain reduction of oxygen valence from 2, common for oxides, down to 1.5 [2]. Combining theoretical simulations with experiment and broadly varying external parameters, pressure, temperature and composition we have discovered several novel nitrides [3-5]. Here, we pay attention to one of the major challenges of the high-pressure synthesis in terms of applications: the need to recover the synthesized material at ambient conditions. We demonstrate feasibility of the approach for the case of metallic, ultraincompressible and very hard rhenium nitride pernitride Re2(N2)(N)2, discovered at pressures from 40 to 90 GPa. In agreement with our theoretical prediction, it has been recovered at ambient conditions, and a route to scale up its synthesis has been developed [4]. Finally, considering the triclinic phase of beryllium tetranitride tr-BeN4 we demonstrate that the high-pressure synthesis can be used in a search for layered materials, precursors of novel 2D-materials. Indeed, BeN4 monolayer, the beryllonitrene, represents a qualitatively new class of 2D materials that can be built of a metal atom and polymeric nitrogen chains and host anisotropic Dirac fermions [5].

[1] E. Bykova, et al., Nature Commun. 9, 4789 (2018). [2] E. Koemets, et al., Phys. Rev. Lett. 126, 106001 (2021), manuscript in preparation. [3] M. Bykov, et al., Angew. Chem. Int. Ed. 59, 10321 (2020); ACS Nano 15, 13539 (2021). [4] M. Bykov, et al., Nature Commun. 10, 2994 (2019). [5] M. Bykov, et al., Phys. Rev. Lett. 126, 175501 (2021)

Hosts: Nils Brouwer

https://xfel.zoom.us/j/96999051414?pwd=R041b2p1WHRsRHlXODZsc2pOTW4rdz09
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