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Melting and metallization of compressed hydrogen: Predictions from first-principles calculations[1]

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A long-sought goal in condensed matter physics has been the metallization of compressed hydrogen. So far, it has been achieved only in the fluid phase at high temperature. In this talk, I will discuss recent results predicting the melting line and a first-order liquid-liquid phase transition from molecular to dissociating fluid in compressed hydrogen [1]. The phase boundaries are computed from first principles using molecular dynamics. The results indicate that there is a maximum in the melting curve of hydrogen and open up the interesting possibility of finding a low-temperature metallic fluid at pressure around 400 GPa. The existence of a maximum melting temperature is rather unusual for a close-packed solid structure. Our analysis indicates that in hydrogen it is a result of changes in intermolecular interactions, occurring in the fluid phase at high pressure. S. A. Bonev, E. Schwegler, T. Ogitsu and G. Galli, *Nature* **431**, 669-672 (2004).

[1]Work performed in collaboration with LLNL under the auspices of the US DOE under contract no W-7405-Eng-48.