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First principles predictions of NaH_x ($x=2-6$) at high pressures
PIO BAETTIG, EVA ZUREK, SUNY at Buffalo — In the last several years, the prediction of novel structures of materials in normal conditions and under pressure has become possible due in part to advances algorithm development. Moreover, the increasing availability of ever faster computers has made it possible to optimize the structures of the materials under investigation in reasonable time frames. In our talk, we will present the application of a genetic algorithm to predict the structures of several potentially superconducting hydrogen rich NaH_x ($x=2-6$) systems. Our work follows up on the recent prediction of LiH_x , ($x=2-8$) which were found to be stable and metallic at 1/4th the pressure required to metallize hydrogen itself.[1] It may be that the addition of Na to H leads the formation of stable, metallic systems at pressures even lower than for LiH_x . We explore which structures are likely to form and be stable, under a wide range of pressures.

[1] E. Zurek, R. Hoffmann, N. W. Ashcroft, A. R. Oganov, A. O. Lyakhov, Proc. Natl. Acad. Sci. **106**, 17640-17643 (2009).

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