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Novel Hydrogen Rich Phases under Pressure

This talk will cover the stabilization of solid phases with unusual combinations or stoichiometries, and unexpected electronic structures that may be achieved by applying external pressure. The prediction of these structures using our chemical intuition (developed at 1 atmosphere) would be exceedingly difficult, making automated structure search techniques prudent. For this reason, we have written XtalOpt, an open-source evolutionary algorithm for crystal structure prediction.

Whereas at 1 atmosphere the classic alkali hydrides combine in a one-to-one ratio, M+H-, under pressure non-classic stoichiometries MHn (n>1) are preferred. For example, theoretical work has predicted that LiH6 and LiH2 become particularly stable phases at about 100 GPa. NaH9 is shown to be the most stable combination of Na and H by 25 GPa. And the rubidium polyhydrides become viable at the industrially achievable pressure of only 2 GPa. These hydrogen-rich materials with nontraditional stoichiometries are computed to undergo an insulator to metal transition at a pressure lower than that necessary to metalize hydrogen. It may be that these systems are superconductors at experimentally achievable pressures.

Eva Zurek's PhD in chemistry (2006) was carried out in the Andersen group in the Max Planck Institute for Solid State Research in Stuttgart, Germany. During this time Eva worked on various topics including: magic clusters, Wannier functions, and the magnetic response of carbon nanostructures. In 2008 she started her postdoctoral work in the group of Nobel Laureate Roald Hoffmann at Cornell University. During this time Eva theoretically examined excess electrons in metal-ammonia systems, and began her studies of solids under pressure. She joined the University at Buffalo, SUNY in 2009 where she is currently an assistant professor. The research in her group focus' on using evolutionary algorithms to predict crystal structures under pressure. New research areas including molecular self-assembly and heterogeneous catalysis are also being pursued.

Wednesday, November 30, 2011
3:30 pm - Room 151, Jorgensen Hall
Refreshments served

Host:
Dr. Axel Enders
Department of
Physics & Astronomy

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