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High-pressure synthesis of materials with new bonding patterns and stoichiometries

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The search for new materials for advanced technological and practical applications requires breakthroughs in our understanding of how we can control matter most efficiently. Pressure is arguably the most revealing physical variable to delineate various competing physical and chemical phenomena. There are multiple theoretical predictions for existence of novel materials state via changes in the equilibrium chemical bonding at high pressures, but many of these reports do not take into account a possible change in the most stable chemical composition. Also, the implications of this novel extreme chemistry for synthesis of new materials for practical applications remain challenging because high-pressure bonding patterns are often thermodynamically unstable at ambient pressure. Search for a recovery mechanisms or attempts of synthesis in nominally metastable conditions require detailed knowledge of the energy landscape; extensive collaborative efforts of experiment and theory are needed for its determination and for validating the theoretical predictions. I will present new results on synthesis of materials with new bonding patterns and unusual stoichiometries containing hydrogen, nitrogen, carbon, sodium, and halogens. This work has been performed in collaboration with M. Somayazulu, V. V. Struzhkin, V. Prakapenka, E. Stavrou, T. Muramatsu, A. R. Oganov, W. Zhang, Q. Zhu, S. E. Boulfelfel, A. O. Lyakhov, Z. Konopkova, H.-P. Liermann, D.-Y. Kim. I acknowledge the support of DARPA, NSF, EFRee (DOE), Army Research Office, Deep Carbon Observatory, and Carnegie Institution of Washington.

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