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Novel compounds synthesized at high pressure-high temperatures

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Pressure undoubtedly tunes inter-atomic and inter-molecular forces far more than any of the other thermodynamic variables. With the rapid advances made in structure prediction techniques, it is therefore not surprising to observe a sudden upsurge in the number of reports of new materials that have richer properties. Concurrently, experimental techniques (especially synchrotron based) have evolved to allow us to measure structures with greater precision and other properties using XAS, NFS and IXS. Such an experimental validation of theoretical predictions has in turn resulted in a search for possible avenues to lower the formation pressure and/or seek metastable means of quenching the HP-HT phases. This talk will highlight all of the above with examples chosen from our work.

Using a combination of pressure and temperature, chemical reactivity between stable salts such as NaCl and KCl and electronegative Cl2 has been predicted. The theoretical predictions point to formation of a number of unexpected phases such as NaCl3, Na3Cl, NaCl7. Using a combination of synchrotron powder diffraction and Raman and IR spectroscopy, experimental validation of these predictions were possible /1/. Similar theoretical predictions on the interaction between chemically inert Xe and Cl2 have postulated that pressure induced hypervalency would drive the transition from van der Waal forces to ionic bonding /2/. This has been verified in the Xe-Cl2 system using a combination of synchrotron powder diffraction and XAS. These results will be presented and to contrast, the discovery of an unexpectedly stable Xe(H2)7 will be presented as also the retrieval of this unique compound to ambient pressure /3/.

With the renewed interest in high temperature superconductivity in hydrides such as H3S, PH3, H3Se, CaH6, YH6, there is a growing interest in synthesis, stability and characterization of these hydrides. While much of the work requires very high pressures and therefore ruling out neutron scattering, a growing body of experimental evidence is bringing out some unexpected formation pathways and structural verifications that serve as an important feedback to theory. The third part of the talk will focus on some of these compounds and how a combination of diffraction and spectroscopy helps unravel the mystery of these ‘super-hydrides’ formed at high pressures.

/1/ Weiwei Zhang et. al., Science (2013), Unexpected Stable Stoichiometries of Sodium Chlorides, 342, 1502
/2/ David Proserpio, Roald Hoffmann and Kenneth Janda, J. Am. Chem. Soc. (1991), The Xe-Cl2 conundrum: van der Waals complex or linear molecule ?, 113, 7184
/3/ Maddury Somayazulu et. al., Nat. Chemistry (2010), Pressure-induced bonding and compound formation in xenon-hydrogen solids, 2, 50-53.

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