Motivation and Goals: We propose to use high pressure to help design and understand new classes of materials suitable for reversible hydrogen storage using a suite of experimental techniques such as Raman and IR spectroscopy, X-ray and neutron scattering and also investigate site specific interactions of storage materials with molecular hydrogen at high pressures. These studies on systems such as NH3BH3-H2; SiH4-CH4-GeH4-H2; Xe-H2 have yielded new compounds and insights into interaction of H2 with other molecular systems.

H2S-H2; SiH4-H2 and GeH4-H2 binary systems – tuning intermolecular interactions with pressure

• CH4+H2
  - Compound formation, small perturbations from bulk molecular hydrogen (Somayazulu et al, Science, 1996)

• SiH4+H2
  - Compound formation, abnormally strong intermolecular interaction with hydrogen (T. Strobel et al, PRL, 2009)

• GeH4+H2
  - Compound formation?

• H2S +H2
  - Host-Guest structure?

Xe(H2)24 – the most hydrogen-rich van der waals solid stable at 90 K and 1 atm.

1. Xe(H2)24 the most hydrogen-rich solid known is stable at 1 atm and 90 K.
2. In comparison to Ar(H2)2 and in fact other binary molecular solids, packing does not seem to play the vital role in this compound formation.
3. First signs of true vdW bonding?
4. Surprisingly, although Xe-H bond formation has been observed at relatively benign P-T conditions, we don’t observe any evidence for Xe-H bond formation even in xenon rich mixtures.
5. At ambient temperatures, no xenon-rich solids are found to occur

Ammonia Borane and related materials

Complexation kinetics much faster (and lower pressure) than AB-H2!

Reaction of ‘clean’ PIB with H2 (2.5 GPa, RT)

Decompose AB to PAB / PIB

H2 Complexes with PAB & PIB


Me2NHBH3/H2 mixtures were found to hydrogenate ethylene and carbon dioxide at room temperature and pressures above 0.5 GPa. Raman spectra of c.a. 4:1 H2:C2H4 before (left) and after (right) reaction. [Potter et al, J. Chem. Phys. (communicated)]

Pressure induced Phase transitions in TMAB.