Successful development of hydrogen as a primary fuel will simultaneously reduce the
dependence on fossil fuel and emissions of greenhouse gases and pollutants. This is
especially critical in this century with increasing concern on energy security and global
warming. Regarding hydrogen storage, one of the major challenges to widespread use of
hydrogen is the lack of suitable hydrogen storage materials with the on-board operating
storage capabilities for fuel-cell vehicular applications. In this talk, I will present some of
our recent work on novel hydrogen storage materials including light-weight complex
metal hydrides (e.g. ammoniates, hydrazinates, and ammonia borane complexes of
borohydrides) and chemical hydrides (e.g. metal ammidoboranes). I will focus on the
structural studies of these materials with aspects of crystal structure determination of
novel hydrides using the combined x-ray powder diffraction and the first-principles
calculation methods. The rich information obtained from the Rietveld structural
refinement analysis and their implications for hydrogen storage will be discussed.