

Seminar Title	: Silicon Nanostructures and its Composites for Solid-state Hydrogen Energy Storage
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Abstract	The sustainable development of hydrogen energy is a prime concern in addressing the rising energy demand and the global energy problem since the hydrogen economy is reliable for clean and carbon-free energy carriers. Despite well-established commercial sector technologies, boil-off losses, explosive nature, and leakage risk still exist with compressed and liquefied storage. One of the significant remedies is solid-state hydrogen storage, which improves bulk density and gravimetric capacity and addresses safety concerns. However, progress toward the hydrogen economy has stalled due to a lack of efficient and economical storage systems, usually restrained by the material used. The work focuses on the importance of existing porous materials for solid-state hydrogen storage and Si nanostructures (SiNSs). Nanostructuring of hand-grinded porous silicon (HGPS) decreases the crystallite size, increases the specific surface area and surface energy, and thereby modifies the thermodynamic properties of the material. At pressures up to 20 bar, HGPS exhibited poor hydrogen uptake, reaching only $0.101 \text{ wt.}\%$ at 120°C. The kinetic models indicate that the storage is in a surface-controlled diffusion stage (α-phase) at 20 bar, with the modified surface providing ample active space for storage at elevated pressure. At 80 bar charging pressure, the ball-milled PS (BMPS) exhibits a hydrogen storage capacity of 10.7 wt.%. The optimized hydrogen uptake capacity in BMPS is 2 wt.% to 6 wt.% for a pressure range of 40 bar to 60 bar, satisfying the Department of Energy (DOE) target of $\sim 5.5 \text{ wt.}\%$. The synergetic effect of PS as the host storage material and Ni as the catalyst in the composite form improves the adsorption rate and reduces the desorption temperature. Due to the catalytic effect of Ni on PS, the average decomposition energy requirement reduces, facilitating desorption at a lowered temperature of 268°C. However, the high atomic mass of Ni leads to a reduced gravimetric capacity in the PS-Ni composition compared to BMPS. The pressure-composition isotherms (PCI) reveal hydrogen storage capacities of $\sim 6.53 \text{ wt.}\%$ for the TrGO+PS composition (where TrGO is Thermally Reduced Graphene Oxide) and $\sim 2.43 \text{ wt.}\%$ for the TrGO+PS+Ni composition. Despite the decrease in weight percentage of TrGO+PS+Ni due to the higher Ni content, dissociation enhances the adsorption rate from 0.35 to $0.53 \text{ wt.}\%$. This study involves modifying the hydrogen storage properties and thermodynamic characteristics of LiH through mechanical alloying with PS. Ten cycles of hydrogenation and dehydrogenation were conducted to evaluate cyclic stability and phase significance. During the first cycle, the composite absorbed $\sim 4.2 \text{ wt.}\%$ hydrogen within 6 min (at 400°C and $\sim 3.8 \text{ MPa}$). It shows a slight 0.11 wt.% capacity drop after ten cycles, confirming its significant stability. Hydrogen absorption and desorption enthalpies of $94.5 \text{ kJ (mol H}_2\text{)}^{-1}$ and $114.9 \text{ kJ (mol H}_2\text{)}^{-1}$ demonstrate the lowest energy demand among previously reported LiH alloys. The evaluation may enable energy providers and Si-based fuel cells and reactor building to be better customized, promoting the development of on-board hydrogen energy applications.