# Donor-Acceptor Stabilization in Main Group Elements: A Computational Study

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POSTER

Recently, much synthetic effort has been placed in attempting to prepare low oxidation state main group hydrides. Primarily, this has been accomplished by using a combination of N-heterocyclic carbenes (electron donors) and Lewis acids (electron acceptors) to stabilize the reactive hydride species.[1] The motivation for carrying out such work has been due to the role of $SiH_2$ as an intermediate species in forming semi-conducting silicon surfaces for use in the electronics industry. However, this approach has also been effective in producing stable hydrides of Ge and Sn. Recently, germanium nanocrystals (GeNCs) with tunable size were synthesized by thermolysis of a Wittig reagent stabilized $GeH_2$ species.[2] These germanium nanocrystals serve to be potentially useful in solar cells, lithium-ion batteries, and biological imaging applications.

In our present work, we have computationally studied both Group 14 hydrides and boron nitride containing compounds when trapped by the ligand $Cy_2BC_6H_4P^iPr_2$ (Cy = cyclohexyl; $^i$Pr = iso-propyl). Interestingly, this ligand contains both Lewis acid and Lewis base functionalities and can be recycled when released upon heating. To study the stability of these compounds, we have carried out ab-initio quantum chemistry computations using density functional theory. These computations have suggested that we can successfully prepare stable Si, Ge and Sn dihydrides as well as a precursor to boron nitride by utilizing this ligand. Boron nitride is of particular interest due to its excellent thermal and chemical stability which makes it suitable for use in the electronics industry as a high temperature insulator.

References:

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