

## ABSTRACT

The discovery of fullerene by Kroto et al lead to the realization that atoms can be caged inside fullerene. The caging of fullerene has great importance due to the fact that hydrogen economy needs efficient storage devices in order to be fully deployed. Till today there are 2-57 reported hydrogen atoms that can be caged inside fullerene. In this study we used car parinello ab initio molecular dynamics with the use of CPMD software. GRID infrastructure of AUTH was used for the computational demands. We used 2, 16, 26, 38, 50, and 58 hydrogen atoms. Fullerene hydrids were studied in 122 K and 300 K which are the Mars planet extreme temperature. MD's were deployed at NVT ensemble.

The maximum calculated capacity of fullerene in hydrogen was 50 atoms at 122 K. Temperature plays critical role because at 50 hydrogen atoms at 300 K the fullerene fails. Moreover the for more than 50 hydrogen atoms the fullerene fails as storage device for both temperatures. The failure mechanism is also described with the help of ab initio molecular dynamics.