

Abstract Submitted
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Hydrogenated silicon fullerenes and endohedral dopings VI-JAY KUMAR, IMR, Tohoku Univ. Sendai Japan and VKF, Chennai, India, YOSHIYUKI KAWAZOE, IMR, Tohoku Univ. Sendai, Japan, - COLLABORATION — Empty cage fullerene structure of Si_{20} can be stabilized by hydrogen capping in equi-atomic concentration [1]. We study hydrogenated silicon fullerenes Si_nH_n , ($n = 14-28$) using *ab initio* ultrasoft pseudopotential method and generalized gradient approximation for the exchange-correlation energy. It is found that $\text{Si}_{20}\text{H}_{20}$ has the optimal size. The empty space in the cages can be filled with atoms and this allows the formation of endohedral silicon fullerenes. The interaction of the guest atom with the cage is weak as compared to metal encapsulated silicon clusters [2]. Our results show that doping can be used to manipulate the highest occupied-lowest unoccupied molecular orbital gaps of these fullerenes and prepare species with large magnetic moments and varied optical properties. Guest atoms with closed electronic shell configurations generally occupy the center of the cage while open shell atoms tend to drift towards the wall of the cage. [1] V. Kumar and Y. Kawazoe, Phys. Rev. Lett. 90, 055502 (2003). [2] V. Kumar and Y. Kawazoe, Phys. Rev. Lett. 87, 045503 (2001).

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