

Abstract Submitted
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Investigation of Trapping Positions for Beryllium Atom in C₆₀ Fullerene and Electron Densities at ⁷Be Nucleus. LEE CHOW, ARCHANA DUBEY, H.P. SAHA, UCF Orlando, GARY S. COLLINS, Washington State University, Pullman, R.H. SCHEICHER, Uppsala University, Sweden, N.B. MAHARJAN, Tribhuvan University Nepal, SUNY Albany, S.R. BADU, R.H. PINK, M.B. HUANG, SUNY Albany, T.P. DAS, SUNY Albany, UCF Orlando — We are investigating, using first-principles Hartree-Fock Roothaan procedure, the trapping sites for ⁷Be atom in C₆₀ Fullerene, following broadly the same procedure as in earlier work by our group for trapping of muonium [1]. A number of possible sites, including the center of the C₆₀ and various positions near the fullerene surface both outside and inside C₆₀ are being studied including the effect of relaxation in the positions of neighboring C atoms. Electron densities at the ⁷Be nucleus will be presented for the sites where the binding energy is positive to attempt to understand the observed anomalous electron capture rate compared to other systems where trapped ⁷Be atom has been studied [2]. Results of our investigations for ⁷Be atom in graphite and graphene will also be presented for comparison with ⁷Be in C₆₀. Possible influence of many-body effects will be discussed. [1] O. Donzelli, T. Briere, T.P. Das, Sol St. Comm. 90 663(1994), Indian J. Phys. 67(Special Issue) 35 (1993) [2] Ohtsuki et al, Phys. Rev. Lett. 93,112501, (2004)

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