

Abstract Submitted
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Theoretical Studies of ground state and photoionization dynamics of Na_x inside C_n ($x=20$ and $n=240$)¹ HARI VARMA RAVI, RASHEED SHAIK, School of Basic Sciences, IIT Mandi, Mandi, Himachal Pradesh 175075, HIMADRI CHAKRABORTY, Department of Natural Science, Northwest Missouri State University, Maryville, Missouri 64468, USA — A number of studies has already been reported on the photoresponse of Na [1] clusters and fullerenes [2]. The hollow space inside fullerene cages can accommodate small metal clusters [3, 4] to form exotic cluster endofullerene molecules. In this work, the ground state of such an endohedral system is modelled in a jellium-based density functional method with a gradient corrected exchange-correlation functional (LB94) [5] before calculating the system's photoionization in a linear response framework called time-dependent local density approximation (TDLDA) [2]. Plasmon and confinement resonances are found to be the key features of the photoionization cross-sections of the system. Comparisons with free systems, Na_x and C_n , facilitate detailed understandings of the results. **References** [1] Chunlei Xia, Chunrong Yin, and Vitaly V. Kresin, Phys. Rev. Lett. 102, 156802 (2009). [2] J. Choi et al., Phys. Rev. A 95, 023404 (2017). [3] Cabrera-Trujillo et al., Phys. Rev. B 53, 16059 (1996). [4] Cabrera-Trujillo et al., Current Problems in Condensed Matter (1998), pp 133-141, Springer, Boston, MA [5] R. van Leeuwen and E. J. Baerends, Phys. Rev. A 49, 2421 (1994).

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