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Effects of exchange-correlation functionals on the structure and the photoionization dynamics of Na_{40} cluster[1] RASHEED SHAIK, HARI VARMA, Indian Institute of Technology Mandi, India, HIMADRI CHAKRABORTY, Northwest Missouri State University, Maryville, USA — Over the years, time-dependent density functional theory has emerged as a powerful tool to study photoionization dynamics of many-electron systems such as atomic clusters [1,2,3]. The accurate prediction of the system's dynamical response to external radiations depends on the accuracy of the form of exchange-correlation functional (xc) used within a density-functional formalism [3]. For spherical Na_{40} cluster, we apply two well known implementations of xc functional in the framework of time-dependent local density approximation (TDLDA), with the Gunnarsson-Lundqvist parametrization [4] for the correlation term. These are: (i) the electron self-interaction correction (LDA-SIC) by Perdew and Zunger [5] and (ii) the van Leeuwen and Baerends model potential (LDA-LB94) [6]. The results obtained by these two schemes will be compared in determining their effects on the ground state structure and the photoionization properties of the system. [1] E. Runge and E. K. U. Gross, *Phys. Rev. Lett.* **52**, 997 (1984); [2] Choi *et al.*, *Phys. Rev. A* **95**, 023404 (2017); [3] Onida *et al.*, *Rev. Mod. Phys.* **74**, 601 (2002); [4] O. Gunnarsson and B. I. Lundqvist, *Phys. Rev. B* **13**, 4274 (1976); [5] J.P. Perdew and A. Zunger, *Phys. Rev. B* **23**, 5048 (1981); [6] R. van Leeuwen and E. J. Baerends, *Phys. Rev. A* **49**, 2421 (1994).

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