Abstract Submitted
for the DAMOP20 Meeting of
The American Physical Society

Exploring the effects of exchange-correlation functionals on the photoionization dynamics of Na_x = ($x = 20, 40 and 92$) clusters[1] HARI VARMA RAVI, RASHEED SHAIK, School of Basic Sciences, IIT Mandi, Mandi, Himachal Pradesh 175075, India, HIMADRI CHAKRABORTY, Department of Natural Science, Northwest Missouri State University, D.L. Hubbard Center for Innovation, Maryville, Missouri 64468, USA — The photodynamics of metal clusters modelled as super-atoms can be studied using a linear-response density-functional method known as the time-dependent local-density approximation (TDLDA) [1]. In this method, the proper choice of exchange-correlation functional (xcf), that appropriately models bound and continuum electron's long-distance properties, is crucial. In the current work, two approximation schemes of xcf with Gunnarsson-Lundqvist parametrization [2] are employed: (i) the electron self-interaction correction scheme [3] and (ii) the Leeuwen-Baerends (LB94) model based on the electron density-gradient [4]. Results determine the role of xcf in the ground state and photoionization description of Na_x (x=20, 40 and 92) clusters. Comparisons of the ionizing residue of plasmon resonances obtained by these xcf schemes with available experimental data will be presented. **References** [1] J. Choi et al., Phys. Rev. A 95, 023404 (2017). [2] O. Gunnarsson and B. I. Lundqvist, Phys. Rev. B 13, 4274 (1976). [3] J.P. Perdew and A. Zunger, Phys. Rev. B 23, 5048 (1981). [4] R. van Leeuwen and E. J. Baerends, Phys. Rev. A 49, 2421 (1994).

[1]National Science Foundation grant PHY-1806206 and SERB EMR/2016/002695

Hari Varma Ravi
School of Basic Sciences, IIT Mandi, Mandi, Himachal Pradesh 175075, India

Date submitted: 04 Jun 2020 Electronic form version 1.4