**DFT+DMFT study of Pressure dependent Insulator-to-Metal transition in molecular *J*eff = 3/2 Mott insulator, GaTa4Se8**

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The lacunar spinel compound GaTa4Se8 is known as the molecular Mott insulator, exhibiting insulator-to-metal transition (IMT) and superconductivity at near 5GPa and 10GPa [1-3]. With first-principles density functional theory (DFT) study shows that spin-orbit coupling (SOC) induce the *J*eff = 3/2 ground state in 4*d*/5*d* series of lacunar spinel compounds [4]. Recent resonant inelastic X-ray scattering (RIXS) experiments established the spin-orbit entangled *J*eff = 3/2 electronic structure [5]. In this study, we performed DFT + DMFT calculations with exact diagonalization (ED) solver [6] to understand IMT under the pressure and role of the SOC. Using the realistic Hubbard *U* parameter from constrained RPA [7], we found that the formation of the *J*eff = 3/2 states with reasonable SOC is essential to reproduce IMT under the high pressure.

[1] M.M. Abd-Elmeguid *et al.* PRL **93**, 126403 (2004)

[2] R. Pocha *et al.* PRL **110**, 037401 (2013)

[3] A. Camjayi *et al.* PRL **113**, 086404 (2014)

[4] H.-S. Kim *et al.* Nat. Commun. **5**, 3988 (2014)

[5] M. Y. Jeong *et al.* Nat. Commun. **8**, 782 (2017)

[6] A. Go, G. S. Jeon. J. Phys.: Condens. Matter **21**, 48 (2009)

[7] S. W. Jang *et al.* Sci. Rep. **6**, 33397 (2016)