Supplementary Information (SI) for Journal of Materials Chemistry C. This journal is © The Royal Society of Chemistry 2024

Supplementary Information for "Intrinsic Magnetism in Semiconducting Bulk Amorphous Tellurium"

Jongchan Kim^{1,2}, Myung Mo Sung² and Kyeongjae Cho^{1*}

¹Department of Materials Science and Engineering, University of Texas at Dallas, Richardson, Texas 75080, USA

²Department of Chemistry, Hanyang University, Seoul 04763, Republic of Korea

*To whom correspondence should be addressed. E-mail: kjcho@utdallas.edu



Figure S1. Band structure and orbital-resolved projected density states (PDOS) of crystalline Te. The inset in (a) represents the high-symmetric *k*-points within the first Brillouin zone of crystalline Te.



Figure S2. Electron localization function (ELF) distribution. (**a**,**b**) In crystalline Te (c-Te), ELF distributions overlap at an isosurface level of 0.47 (a) and intensify at 0.43 (b). (**c**,**d**) In amorphous Te (a-Te), no overlap is observed at 0.47 (c), but overlap occurs at the lower ELF level of 0.43 (d), indicating localized behavior and partial bond breaking in a-Te.