Angle-Resolved Photoemission Calculations of WTe_2 Compared to Experiment

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Abstract. Molybdenum dichalcogenides are probably the most studied single layer TMDCs by virtue of being appealing for sundry possible applications suchlike transistors, diodes, solar cells or more fundamental studies of spin or valley pseudospin and their interactions. Tungsten-based counterparts are on the other hand evincing much stronger spin-orbit coupling due to which all the spin-related effects are more stable at room temperature and thus more feasible for application. WTe_2, a type-II Weyl semimetal is in particular interesting due to having two pairs of spin-differentiated Weyl points above Fermi energy. We have conducted several experiments following the evolution of the band dispersion in the vicinity of X and Y points of the Brillouin zone of WTe_2 which is substantial for understanding the fundamental properties of the structure-property relation of the system. Ab-initio set of photoemission calculations was performed using SPR-KKR package and compared to experimental results.