Theoretical and Experimental Soft X-Ray Photoemission Study of Weyl-Semimetal TaAs

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Abstract. A Weyl semimetal is a new matter state possessing Weyl fermions near the Fermi level with several unique physical properties and it is confirmed by the existence of Fermi arc surface states [1]. In this work we study tantalum arsenide (TaAs) which is a prototypical Weyl semimetal compound. The electronic structure properties have been studied by soft and hard X-ray angle-resolved photoemission spectroscopy (ARPES) at energies of 440 eV and 2150 eV, respectively. For the first time, TaAs is experimentally investigated by the bulk sensitive photoemission in the hard X-ray regime. In order to interpret experimental data we performed one-step model of photoemission calculation which includes all matrix elements and final state effects [2,3,4]. Due to the strong photon momentum effects and uncertainty in the tilt of experimental geometry we used machine learning procedure combined with a free-electron final-state model to find best possible experimental parameters. Our findings re-emphasize the overwhelming accuracy of hard X-ray ARPES compared to the traditional ultraviolet and soft X-ray one in case of bulk electronic structure, motivating further material discoveries.

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