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Optical evidence for bonding-antibonding splitting in $IrTe_2$ DIPANJAN MAZUMDAR, Southern IL Univ-Carbondale,USA, KRISTJAN HAULE, Rutgers University, Piscataway, USA, J.J YANG, Laboratory for Pohang Emergent Materials and Department of Physics, Korea, G.L. PASCUT, Rutgers University, Piscataway, USA, B.S. HOLINSWORTH, K.R. O'NEAL, University of Tennessee, Knoxville, USA, VALERY KIRYUKHIN, SANG-WOOK CHEONG, Rutgers University, Piscataway, USA, J.L. MUSFELDT, University of Tennessee, Knoxville, USA, DEPARTMENT OF CHEMISTRY, UNIVERSITY OF TENNESSEE, KNOXVILLE, USA TEAM, DEPARTMENT OF PHYSICS AND ASTRONOMY, RUTGERS UNIVERSITY, PISCATAWAY, USA TEAM, LABORATORY FOR POHANG EMERGENT MATERIALS AND DEPARTMENT OF PHYSICS, POHANG, KOREA TEAM, RUTGERS CENTER FOR EMERGENT MATERIALS, RUTGERS UNIVERSITY, USA TEAM, SOUTHERN ILLINOIS UNIVERSITY, CARBONDALE, USA TEAM — We combined optical spectroscopy with first principles calculations to reveal the electronic signatures of Ir dimer formation in the 1/5th phase of IrTe2. Our measurements uncover two interband transitions into the unoccupied dxy anti-bonding orbital, one from mixed Iridium/Tellurium bands, the other from the dxy bonding orbital of the dimerized Ir centers. The bonding-antibonding splitting demonstrates that Iridium, not Tellurium, plays the dominant role in stabilizing the low temperature phase of IrTe2 through localized bonding orbital formation.

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