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Dimerization-Induced Cross-Layer Quasi-Two-Dimensionality in Metallic Iridate $IrTe_2$ GHEORGHE-LUCIAN PASCUT, KRISTJAN HAULE, Rutgers University, NJ, USA, MATTHIAS J. GUTMANN, ISIS, UK, SARAH A. BARNETT, ALESSANDRO BOMBARDI, Diamond, UK, SERGEY ARTYUKHIN, TURAN BIROL, DAVID VANDERBILT, Rutgers University, NJ, USA, JUNJIE YANG, Pohang University of Science and Technology, Korea, SANG-WOOK CHEONG, VALERY KIRYUKHIN, Rutgers University, NJ, USA — $IrTe_2$ a layered chalcogenide metal composed of stacked layers of $IrTe_6$ octahedra, has recently received a lot of interest due to: (1) the structural phase transition (T_S =280 K) to a modulated structure characterized by the wave vector $\boldsymbol{q_0}$ =(1/5, 0, 1/5) and (2) the superconducting properties of the Pd/Pt-doped/intercalated samples. Using the crystal structure obtained from single crystal X-ray diffraction and first principle calculations we show that the mechanism for the structural phase transition is driven by the Ir dimerization and bonding, contrary to mechanisms proposed before based on: orbital-driven Peierls instability, crystal field splitting the Te p orbitals and depolymerization of the inter-layer Te bonds. In this talk I will describe the Ir/Te dimers and the electronic structure calculations which reveal an intriguing quasi-two-dimensional electronic state, with planes of reduced density of states cutting diagonally through the Ir and Te layers. These planes are formed by the dimers exhibiting a signature of covalent bonding character development. The role of the electronic correlations and spin orbit coupling will be also discussed.

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