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Surface Structure and Work Function of ZnO Based on First Principle DFT Calculations YUN LI, JINCHENG DU, UNT — Zinc Oxide is a well known n-type wide band gap semiconductor material and remains actively as a strategic material for various photonic applications. The fabricate ZnO, is effectively used as a sensor in various applications, Because of its high infrared reflectance and high visible transmittance. Due to that fact, its electron property plays vital role and attract our attention. Via simulation method, their electron properties were studied through density function theory. Based on first principle theory, their structures with distinct cleaved planes were obtained and completed relaxed in DFT based methods. Depending on cleaved planes, there were Oxygen or Zinc atoms terminated along (001) direction and both of them locating on the cleaved surface (110). Work function and other electron properties will be discussed in detail for all of them and compared with the experimental values, the difference and prediction will be made.

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