

# Theoretical investigation of the Zinc Oxide ZnO: Ground and Excited States

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## **Abstract:**

Zinc is a chemical element known for its applications in many fields (environment, cosmetics, pharmaceuticals, nutritional additives, it is considered important because of the major role it plays in many enzymatic reactions indispensable to the life of living beings, Recent research has shown that zinc oxide also has the same importance except that the complicity of its spectra and electronic structure entangled makes its study by experimenters and theorists difficult.. Solving equations based on the construction of approximate wave functions for ZnO systems, followed by a study of this compound by the Variable Multireference [MRCI] and Coupled Cluster Methods [RCCSD (T)] using augmented bases. Obtained from these calculations will be compared with the experimental results.