

AB INITIO CALCULATIONS OF THE GROUND AND EXCITED STATES OF THE ZNTE MOLECULE AND ITS IONS ZnTe^+ AND ZnTe^-

NOUR EL HOUDA BENSIRADJ, OURIDA OUAMERALI, AZEDDINE DEKHIRA, *Laboratory lctcp, University USTHB, Algiers, Algeria*; TIMÓN VICENTE, *Molecular Physics, Instituto de Estructura de la Materia (IEM-CSIC), Madrid, Spain*.

The ZnTe system exhibits very interesting optoelectronic properties. It is a promising candidate for the development of detectors of Terahertz (THz) radiation, as well as a growing number of applications, particularly in the area of radiology.

In this work, we report a theoretical study of the ground state and various excited states of ZnTe and its ions ZnTe^+ and ZnTe^- . The potential energy curves are calculated using CASSCF method, as implemented in Molpro. These curves serve to determine the different spectroscopic constants such as the internuclear distance (R_e), the harmonic vibration frequency (ω_e), the rotation constant (B_e) and the dissociation energy (D_e). The results obtained are in good agreement with the available experimental data.