GROUND AND EXCITED STATES OF PLATINUM DIMER: TIME-DEPENDENT RELATIVISTIC DENSITY FUNCTIONAL THEORY STUDY

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Platinum dimer has been studied using DFT and TDDFT methods, at B3LYP and BLYP levels, respectively. Segmented all-electron relativistically contracted in conjunction with the DouglasKrollHess (SARC-DKH) basis sets were used which include scalar relativistic effects. First, the potential energy curves are obtained and the properties of the ground state are discussed briefly. The fully optimized bond length and the calculated dissociation energy are compared with the results obtained from non-relativistic calculations and from experiment. The electronic structure of the ground and three low-lying excited states are also examined.