XIX SBQT
Simpósio Brasileiro de Química Teórica 2017
12 a 17/Nov, 2017, Águas de Lindóia/SP, Brasil

Ground State Energy for Confined Hydrogen Molecule

Hugo de Oliveira Batael*, Elso Drigo Filho

Universidade Estadual Paulista "Júlio de Mesquita Filho", Campus São José do Rio Preto, Instituto de Biociências, Letras e Ciências Exatas
**email:hugobatelll@gmail.com*

Abstract: The ground state energy for the confined H_2 molecule is computed by the Variational Method [1]. The approach proposed here uses the wave function molecular of the type Valence Bond (VB) [2], written as the sum of the covalent term with ionic term, for last term is given a weight different in relation the first term. The molecule is confined in impenetrable prolate spheroidal boxes. The atomic orbitals are built from previous suggestion inspired from the factorization of Schrödinger equation [3]. The aim of this work is to propose a simple wave function for confined hydrogen molecule, compared with wave functions found in literature [4]. The results obtained are in agreement with other results presents in the literature.

Key-words: **Molecular Confinement, Hydrogen Molecule, Variational Method.**
Support: This work has been supported by CAPES and FAPESP
References:
[1] Schiff, L. I.; Quantum Mechanics. 3. ed. New York: Mcgraw-hill, 1968
[2] Levine, I. N.; Quantum Chemistry, Prentice Hall, New York, USA, 1991.
[3] Drigo Filho, E.; Ricotta, R. M.; Phys. Lett. A 2002, 299, 137.
[4] Colín-Rodríguez, R.; Cruz, S. A.; J. Phys. B: At. Mol. Opt. Phys. 2010, 43, 235102.