

Abstract Submitted  
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**First-Principles Hartree-Fock-Roothaan Study of Ground State of Ozone including Many-Body Effects** SHEKHAR GURUNG, M.M. ARYAL, D.D. PAUDYAL, D.R. MISHRA, N.B. MAHARJAN, B. DHAKAL, Central Dept. of Physics, Tribhuvan University, Kathmandu, Nepal, R.H. SCHEICHER<sup>1</sup>, JUNHO JEONG, T.P. DAS<sup>2</sup>, Dept. of Physics, SUNY at Albany, NY — Earlier investigations<sup>3</sup> by our group on the ground state of Ozone molecule have shown a sensitive dependence of the binding energy on the size of the variational basis set used and the treatment of many-body effects. We have recently carried out new investigations using some of the most extensive basis sets available for Oxygen atom including many-body effects through both perturbation procedure upto fourth order and configuration interaction. Results will be discussed for the total energy, binding energy and geometry of the ground state and excitation energy for the singlet isomeric state with equilateral triangle structure.

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<sup>3</sup>[www.aps.org/meet/march03/H12.009](http://www.aps.org/meet/march03/H12.009)

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