Abstract Submitted for the MAR07 Meeting of The American Physical Society

Quantum Monte Carlo studies of transition metal atoms and molecules RYO MAEZONO, Computational Materials Science Center, National Institute for Materials Science, Japan, LUCAS K. WAGNER, MICHAL BAJDICH, JINDRICH KOLORENC, LUBOS MITAS, North Carolina State University — We study electron correlation in selected transition metal atoms and molecules from the 3d series by variational and fixed-node diffusion Monte Carlo methods. We test several types of orbitals such as RHF, UHF, B3LYP and atomic natural orbitals in building the Slater determinants. We explore also several types of wave functions based on single determinant, GVB, limited CI expansions with both unoptimized and reoptimized weights. The aim of this study is to estimate the accuracy of various wave functions with regard to fixed-node biases and to provide benchmarks for high accuracy calculations with these types of atoms.

> Ryo Maezono Computational Materials Science Center, National Institute for Materials Science, Japan

Date submitted: 13 Nov 2006

Electronic form version 1.4