Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

A quantum Monte Carlo study of molecular systems with heavy elements SHI GUO, KEVIN RASCH, LUBOS MITAS, North Carolina State University, ENRIQUE BATISTA, RICHARD MARTIN, Los Alamos National laboratory — We use quantum Monte Carlo method to study the bis-cyclopentadienyl Hafnium dichloride molecule Cp_2HfCl_2. There are two Cl dissociation channels for Cp_2HfCl_2: one is to break into neutral fragments, the other one into charged fragments. We employ the Stuttgart pseudopotential to represent the Hf atom and optimized Slater-Jastrow trial wave function at the variational Monte Carlo level. The calculations of the dissociation energies are carried out by the fixed-node diffusion Monte Carlo. We observe that for the heavy elements the low valence density in the core region can generate large energy fluctuations and we address this by improvements of the correlation factor. Alternatively, we construct Hf pseudopotentials with different core sizes and test for the accuracy of such pseudopotential Hamiltonians. We compare the QMC results also with DFT calculations with hybrid functionals.

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Date submitted: 18 Nov 2010 Electronic form version 1.4