Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Modeling Electron Correlation Using Geminal Hybrid Methods[1]
BRETT CAGG, VITALY RASSOLOV, University of South Carolina — Two approaches to dynamic correlation correction for a variationally optimized, spin-unrestricted, multireference wavefunction based on strongly orthogonal, two electron geminals are presented. The first is a simple density functional based approach using standard correlation functionals rescaled empirically to reduce the correlation double counting error (DCE) inherent in all multireference DFT approaches. The second uses a two electron correlation operator to correlate only intergeminal, mean-field type, interactions within the wavefunction and effectively eliminates DCE. The performance of each is examined by geometric optimization and dissociation energy prediction of 38 diatomic molecules at two different basis sets.

[1]NSF grants CHE 1048629 and CHE 1213604

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Date submitted: 13 Nov 2013 Electronic form version 1.4