

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Auxiliary field quantum Monte Carlo study of transition metal and post-d group atoms and molecules¹ HENRY KRAKAUER, College of William and Mary, WISSAM A. AL-SAIDI, College of William and Mary, SHIWEI ZHANG, College of William and Mary — We applied the phaseless auxiliary field quantum Monte Carlo [1] to the study of several transition metal and post-d atoms and molecules. The transition metal study includes both all-electron and pseudopotential calculations, while the post-d group elements are studied using the consistent correlated basis which employs a small core relativistic pseudopotential [2]. The obtained electron affinities, dissociation energies, and equilibrium geometries compare favorably with experiment and with coupled cluster results. [1] S. Zhang and H. Krakauer, *Phys. Rev. Lett.* **90**, 136401 (2003). [2] Kirk A. Peterson, *J. Chem. Phys.* **119**, 11099 (2003); Kirk A. Peterson *et al.*, *J. Chem. Phys.* **119**, 11113 (2003)

¹supported by ONR and DOE/CMSN

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Date submitted: 06 Dec 2005

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