Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Quantum Monte Carlo for the Spectroscopy of Core Excited States DMITRY ZUBAREV, UC Berkeley — X-ray absorption spectroscopy is a powerful experimental tool that is capable of delivering valuable information about very delicate aspects of electronic structure and reveals details of the local chemical environment in many systems of fundamental and applied importance. The rigorous interpretation of core-level spectra requires very accurate quantum chemical simulations. The trade-off between feasibility of treatment of large systems and consistency in description of electron correlation tremendously hinders the generation of accurate theoretical results for many experimental studies. We show that the fixed-node diffusion Monte Carlo (FN-DMC) approach can be used straightforwardly for the accurate simulation of core-level spectra. Basic methodological aspects are addressed, including the strategy for the construction of adequate trial wave functions. Examples of FN-DMC calculations of core-level spectra of water and pyrrole are presented. The possibility of the simulation of X-ray absorption spectra of solvent-solute systems is discussed.

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Date submitted: 29 Nov 2011 Electronic form version 1.4