

Abstract Submitted  
for the MAR17 Meeting of  
The American Physical Society

**Benchmark of Ab Initio Bethe-Salpeter Equation Approach with Numeric Atom-Centered Orbitals** CHI LIU, Department of Chemistry, Duke University, Durham, NC, JAN KLOPPENBURG, Institute of Condensed Matter and Nanosciences, Universit catholique de Louvain, Belgium, YOSUKE KANAI, Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC, VOLKER BLUM, Department of Mechanical Engineering and Material Science, Duke University, Durham, NC — The Bethe-Salpeter equation (BSE) approach based on the GW approximation has been shown to be successful for optical spectra prediction of solids and recently also for small molecules. We here present an all-electron implementation of the BSE using numeric atom-centered orbital (NAO) basis sets. In this work, we present benchmark of BSE implemented in FHI-aims for low-lying excitation energies for a set of small organic molecules, the well-known Thiel’s set. The difference between our implementation (using an analytic continuation of the GW self-energy on the real axis) and the results generated by a fully frequency dependent GW treatment on the real axis is on the order of  $\sim 0.07$  eV for the benchmark molecular set. We study the convergence behavior to the complete basis set limit for excitation spectra, using a group of valence correlation consistent NAO basis sets (NAO-VCC-nZ), as well as for standard NAO basis sets for ground state DFT with extended augmentation functions (NAO+aug). The BSE results and convergence behavior are compared to linear-response time-dependent DFT, where excellent numerical convergence is shown for NAO+aug basis sets.

Chi Liu  
Department of Chemistry, Duke University, Durham, NC

Date submitted: 11 Nov 2016

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