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Ab initio **Bethe-Salpeter Equation approach for aperiodic materials and core-excitations** H.M. LAWLER, J. VINSON, J.J. REHR, University of Washington, E.L. SHIRLEY, NIST — We have recently developed an interface dubbed AI2NBSE between the Bethe-Salpeter optical spectroscopy code NBSE developed at NIST and the *ab initio* electronic structure code ABINIT [1]. This interface facilitates first-principles calculations of valence-band dielectric response including excitonic effects in insulating crystals. Here we report on the extension of this interface for calculations of 1) dielectric response in complex nano-scale, disordered, and molecular systems, and 2) core-level UV and x-ray response. For the treatment of complex systems, we discuss issues of cell selection, basis size, and the treatment of the screened electron- hole interaction. For the core level response, we address various strategies including explicit treatments of core and semi-core states with plane waves and the PAW representation. *Supported by DOE Grant DE-FG03-97ER45623. [1] H. M. Lawler, J. J. Rehr, F. Vila, S. D. Dalosto, E. L. Shirley and Z. H. Levine, Phys. Rev. B **78**, 205108 (2008).

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