Recyclable metal, friends, commoners and cinders—spectroscopic studies in Al, Si, diamond, LiF and MgO

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We will review progress made in the calculation of entire optical constant spectra in a variety of low-Z systems, including innovation reflected in the AI2NBSE and OCEAN packages and DFT calculations based on the 2n+1 theorem. A common thread throughout this work will be the first-principles methodology and the development of practical means to implement approximations. Beginning with DFT ground state calculations, we shall proceed to calculates of the electron self-energy, the screening of core and valence holes, the solution of the two-particle (electron-plus-hole) Bethe-Salpeter equation, and determination of the coupling of phonons and phonon pairs to infrared light. Many of the developments are complementary to and outside the scope addressed by the FEFF project, but the FEFF project has certainly touched on all topics covered. Moreover, the cooperative and collaborative nature of electronic structure methods development that has been necessary for this work's success is certainly well demonstrated by Professor John Rehr.