

## Theoretical calculation of self - consistent optical potential based on $GW$ scheme

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Recently a method for utilizing the near edge part of the absorption spectrum (XANES) for structural analysis has been proposed by Benfatto and Della Longa (*J. Synchrotron Rad.* (2001), 8 , 1087). In this method hundreds of theoretical signals obtained by fully inverting the multiple scattering matrix are compared with the experimental data, until a best fit is obtained in the parameter space of the atomic positions. Very good results are obtained if in the course of the fitting procedure the optical potential used to generate the theoretical signal is taken as the real part of the Hedin-Lundqvist (H-L) potential, whereas for the imaginary part, describing the damping of the excited photoelectron, a suitably parametrised functional form is fitted together with the structural parameters. Indeed the use of the imaginary part of the H-L potential usually leads to fits with bad R-factors. Clearly the fault lies in the single plasmon pole approximation applied also to core electron densities. Following the theory for the optical potential based on the  $GW$  approximation for core electrons as developed by Fujikawa, Hatada and Hedin (*Phys. Rev. B* 62, 5387, 2000), we have studied the performance of this potential, and especially its imaginary part, in the fitting procedure for some significant test cases, namely transition metal ions in water solution. The results of this investigation are hereby presented.