Band structure of plasmonic polarons using the Sternheimer-GW method

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During the past two decades the GW method witnessed significant growth within the electronic structure community. Besides its predictive power in the calculation of quasiparticle band structures, the GW method is appealing since it does not require the use of adjustable parameters. Despite these successes GW calculations suffer from the slow convergence of quasiparticle energies with respect to the number of unoccupied Kohn-Sham states. In order to circumvent this difficulty we developed the so-called 'Sternheimer-GW' method, which avoids the explicit computation of unoccupied Kohn-Sham states [1,2]. In Sternheimer-GW both the screened Coulomb interaction W and the electron Green's function G are evaluated using only occupied Kohn-Sham states, precisely as in density-functional perturbation theory. In this talk I will review the basics of Sternheimer-GW, and discuss comparisons with calculations based on the standard sum-over-states approach. In addition I will discuss one recent application to the calculation of complete energy- and momentum-resolved spectral functions of semiconductors such as three-dimensional bulk silicon and two-dimensional transition metal dichalcogenides. Here, by using Sternheimer-GW in conjunction with the cumulant expansion approach, we have found dispersive photoemission satellites associated with electron-plasmon interactions. The energy vs. momentum dispersion relations of these plasmonic structures closely resemble the standard valence bands, although they are broadened and blue-shifted by the plasmon energy [3].

[1] F. Giustino, M. L. Cohen, S. G. Louie, Phys. Rev. B 81, 115105 (2010).
[2] H. Lambert, F. Giustino, Phys. Rev. B 88, 075117 (2013).
[3] F. Caruso, H. Lambert, F. Giustino, Phys. Rev. Lett. (2015), in press.