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The Sternheimer-GW method and the spectral signatures of plasmonic polarons[1]

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During the past three decades the GW method has emerged among the most promising electronic structure techniques for predictive calculations of quasiparticle band structures. In order to simplify the GW work-flow while at the same time improving the calculation accuracy, we developed the Sternheimer-GW method [1]. In Sternheimer-GW both the screened Coulomb interaction and the electron Green's function are evaluated by using exclusively occupied Kohn-Sham states, as in density-functional perturbation theory. In this talk I will review the basics of Sternheimer-GW, and I will discuss two recent applications to semiconductors and superconductors. In the case of semiconductors we calculated complete energy- and momentum-resolved spectral functions by combining Sternheimer-GW with the cumulant expansion approach. This study revealed the existence of band structure replicas which arise from electron-plasmon interactions [2]. In the case of superconductors we calculated the Coulomb pseudo-potential from first principles, and combined this approach with the Eliashberg theory of the superconducting critical temperature [3]. [1] H. Lambert, F. Giustino, Phys. Rev. B 88, 075117 (2013). [2] F. Caruso, H. Lambert, F. Giustino, Phys. Rev. Lett. 114, 146404 (2015). [3] E. R. Margine, F. Giustino, Phys. Rev. B 87, 024505 (2013).

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