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Ab initio **Sternheimer-GW method for quasiparticle calculations**[1]
HENRY LAMBERT, FELICIANO GIUSTINO, Oxford Univ-USE 4643 — The GW method has emerged as the standard computational tool for investigating electronic excitations in bulk and nanoscale systems. Recently significant efforts have been devoted to extending the range of applicability of the GW method. With this aim, Ref. [1] introduced the Sternheimer-GW method, reformulating the standard GW approach so that no unoccupied electronic states are required in the calculations. Here we present the implementation of the Sternheimer-GW method using planewaves and norm-conserving pseudopotentials [2]. In our method we calculate the complete position- and energy-dependent GW self-energy operator, and as a by-product we obtain the entire G_0W_0 quasiparticle spectral function. We have validated our method by calculating the quasiparticle band structures of standard semiconductors and insulators (Si, SiC, diamond, LiCl) and by comparing the results with previous GW calculations. This method is currently being used for investigating the electronic structure of novel materials of reduced dimensionality.

[1] F. Giustino, M. L. Cohen, and S. G. Louie, Phys. Rev. B **81**, 115105 (2010).
[2] H. Lambert and F. Giustino, Phys. Rev. B. **88**, 075117 (2013)

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