Abstract Submitted
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Satellite Structures in Spectral Functions of Silicon and Graphene from ab initio GW and Cumulant Expansion Calculations[1] DEREK VIGIL CURREY, JOHANNES LISCHNER, STEVEN LOUIE, University of California at Berkeley and Lawrence Berkeley National Lab — The GW approximation is a well-established method for obtaining accurate quasiparticle properties in a wide range of materials. Its suitability for satellite structures (e.g., those measured in photoemission spectroscopies), however, has rarely been addressed in detail for real materials and the fact that GW overestimates the position of the plasmon satellite peaks in the spectral function of silicon indicates the need for an improved method for satellites. One such method is the cumulant expansion. The cumulant expansion is a method that includes, approximately, higher-order processes beyond GW that are important for satellite properties. We present here full-frequency results for the satellite and quasiparticle properties of silicon and doped graphene using the GW and the cumulant expansion methods, and discuss the improvements in satellite properties given by the cumulant expansion. We also compare our results to earlier model calculations on doped graphene.

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