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Ab-initio description of satellites in graphite MATTEO GUZZO, LORENZO SPONZA, CHRISTINE GIORGETTI, FRANCESCO SOTTILE, Ecole Polytechnique, FR, DEBORA PIERUCCI, MATHIEU G. SILLY, FAUSTO SIROTTI, Synchrotron SOLEIL, FR, JOSHUA J. KAS, JOHN J. REHR, U. Washington, LUCIA REINING, Ecole Polytechnique, FR — The GW method from Many-Body Perturbation Theory has been very successful in describing photoemission spectra in a variety of systems. In particular, GW is known to give good quasiparticle properties like band-gaps, but it has shown some limitations in the description of complex correlation effects like satellites. Satellite peaks in photoemission come from higher-order excitations and are still poorly studied in the valence bands. In perturbative GW the spectral function can describe additional features beside the quasiparticle peaks, but these satellites are known to be too weak and too low in energy, as it appears from calculations on the Homogeneous Electron Gas and some real materials. We have recently shown that including additional diagrams in the Green's function (similarly to what has been done with the cumulant expansion) we obtain an excellent description of satellites series in the test case of bulk silicon, where GW is unable to cope. We now focus on a more complex system, i.e. graphite, with this same approach. Using our newly measured XPS valence data, we investigate the effects of anisotropies on satellites and give a prediction on the spectral changes following the transition towards a single graphene layer.

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