The Gamma (and open shell) challenge in GW and BSE calculations

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GW and the Bethe Salpeter are nowadays implemented in many first-principles packages. Their accuracy in predicting charged and neutral excitations has been extendedly demonstrated. With the boom of High Performance Computing and the promise of turn-key solutions in first-principle modelling, why should we still discuss about challenges in GW-BSE?

After a brief introduction on GW-BSE, we will show some examples that rise questions on reproducibility and affordability of GW-BSE calculations, with a particular emphasis in the context of defects in semiconductors and insulators. Indeed, because of the variety in the implementation details and the high computational cost, a simple search on the silicon band gap within GW might lead to finding a variety of numbers. A number is just a number? Should we move towards a standardisation? with which criteria? Or should we better invest in increasing the awareness on what is standing behind the scene?