High-Harmonic Imaging of Spin-Polarised Defects in Solids

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High order harmonic generation (HHG) is a probe useful for understanding the ultrafast electron dynamics in materials, originally developed for atomic and molecular systems. Recently, HHG was realized from solids [1]. Within a decade of its discovery, HHG in solid is getting tremendous attraction due to its capability to explore fundamental physics of solids. Extending the techniques developed originally for atomic and molecular gases to solid state materials requires a fundamental understanding of the physics at place that has been recently only partially addressed theoretically. In the case of strong-field driven electron dynamics in solids, not much is known how the different kinds of defects in solids affect the HHG spectra. Here we employ time-dependent density-functional theory to investigate how the electron dynamics resulting in high-harmonic emission in monolayer hexagonal boron nitride is affected by the presence of point defects. We show how realistic spin-polarised defects modify the harmonic emission, and demonstrate that crucial differences exist between harmonics from a pristine solid and a defected-solid. In particular, we found that the different spin defect-channels are affected differently, and that localisation of the wavefunction, the geometry of the defect and the electron-electron interaction are all important ingredient to describe high-harmonic generation in defected-solids. Our work opens the door to the high-harmonic imaging of spin-polarised defects in solids.

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[1] Ghimire S., DiChiara A.D., Sistrunk E., Agostini P., DiMauro L.F. and Reis D.A., *Nature physics* ***7*****(2)**, 138 (2011).