Simulating the anisotropic spin behavior of graphene induced by proximity to PdSe2

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Abstract

In this work, we conduct a theoretical study of the spin transport properties of graphene when tuned by proximity effects from a PdSe2 monolayer. Motivated by the pursuit of developing novel spin-based memory devices and discovering new ways to engineer spin currents in nanodevices, a recent experimental study has shown that PdSe2 is an outstanding platform for manipulating spin behavior in graphene[1]. Highly anisotropic in nature, the origins of the exotic spin behavior in the PdSe2+Graphene heterostructure remain largely unknown. Particularly intriguing is the fact that the axis of maximum spin relaxation does not match the crystallographic axis. Here, we use Siesta DFT software to generate a model of PdSe2+Graphene and perform several numerical studies in order to investigate this unusual behavior. Using time evolution[2], we explore the spin precession anisotropy with respect to insertion angle. Using Kubo formulas, we directly compute the charge to spin conversion efficiency across the material.

References

[1] Sierra, J.F., Světlík, J., Savero Torres, W. *et al.* Room-temperature anisotropic in-plane spin dynamics in graphene induced by $PdSe_2$ proximity. *Nat. Mater.* **24**, 876–882 (2025). https://doi.org/10.1038/s41563-024-02109-2

[2] Fan, Zheyong & Garcia, Jose & Cummings, Aron & Barrios Vargas, José Eduardo & Panhans, Michel & Harju, Ari & Ortmann, Frank & Roche, Stephan. (2020). Linear scaling quantum transport methodologies. Physics Reports. 903. 10.1016/j.physrep.2020.12.001.

Figures

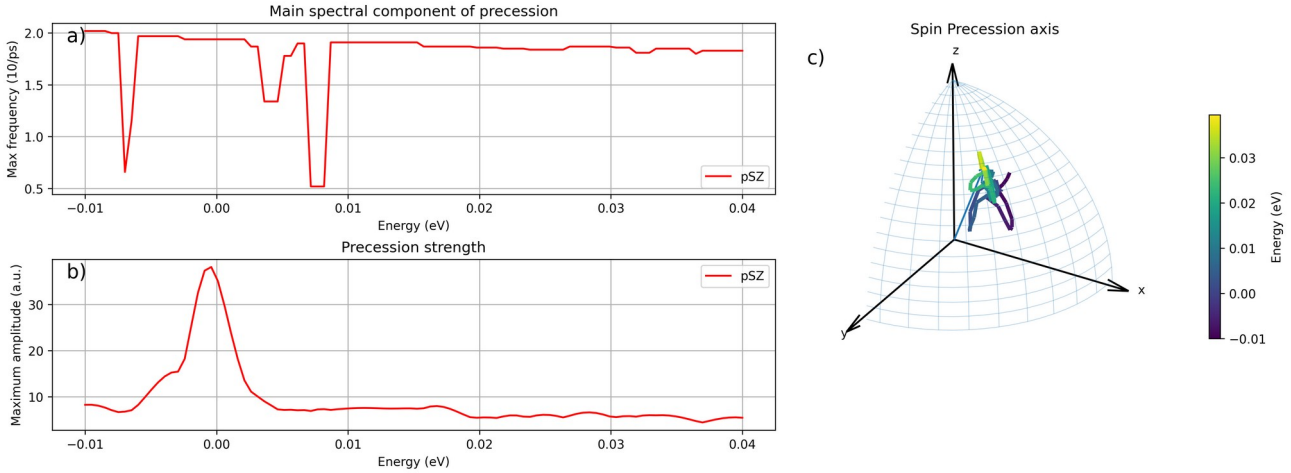

Figure 1: Time evolution study of the spin precession in the DFT graphene+ PdSe2 heterostructure model. a) Spin precession frequency across a range of Fermi energies close to the charge neutrality point. c) Spin precession intensity in the same range of energies d) graphene+PdSe2 structure. b) Spin precession axis direction