NANO COLLOQUIA 2024 - S3 SEMINAR

Generalized density functionals for the electronic structure of spin-orbit coupled states and non-collinear spins

Thursday September 12, 2024 – 14:30

ON-SITE - S3 Seminar Room, Third Floor, Physics Building
ONLINE - https://tinyurl.com/NanoColloquia

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Abstract

Spintronics and topologically non-trivial phases of matter have led to an explosion of interest in spin-orbit interactions. In addition, the recent discovery of altermagnets is writing a new chapter of physics and opening new avenues toward near-future technological exploitations. Consequently, the longstanding call for an extended Density Functional Theory (DFT) for magnetism is receiving a stronger push. At the level of the (two-component) Scrödinger-Pauli equation, Spin-Current-DFT (SCDFT) offers a formally exact framework to handle the treatment of interacting many-electron systems in magnetic fields including spin-orbit coupling (SOC). [1] In practice, robust and accurate calculations of the electronic structure of these systems call for functional approximations that obey additional exact conditions and depend not only on the particle- and spin-densities but also on the particle- and spin-currents and, explicitly, also on the Kohn-Sham spinors. [2]

In this seminar — first focusing on time-reversal symmetric spin-orbit coupled states — I will show how spin-currents can be added non-empirically to meta-Generalized-Gradient Approximations by invoking the SU(2) gauge principle, as for the SCAN form. [3] I will also show by working within a Generalized Kohn-Sham approach for the band structure, that the regular second-variational treatment of SOC is unable to match the self-consistent SCDFT results for the Rashba splittings. [4,5] Second, I will present the extension of the electron localization function — a popular descriptor of molecular bonds and atomic shells, also used in the construction of modern density functional approximations — to non-collinear magnetic states. [6]

[1] "Current- and spin-density-functional theory for inhomogeneous electronic systems in strong magnetic fields", G. Vignale and Mark Rasolt, Phys. Rev. B 37, 10685 (1988);
"Spin–orbit coupling in the spin-current-density-functional theory", K Bencheikh, J. Phys. A: Math. Gen. 36 11929 (2003)

[2] "U(1)×SU(2) gauge invariance made simple for density functional approximations", S. Pittalis, G. Vignale, and F. G. Eich, Phys. Rev. B 96, 035141 (2017)

[3] "Spin-currents via the gauge-principle for meta-generalized-gradient exchange-correlation functionals", J.K. Desmarais, J. Maul, B. Civalleri, A. Erba, G. Vignale, and S. Pittalis, Phys. Rev. Lett. 132, 256401 (2024)

[4] "Generalized Kohn-Sham Approach for the Electronic Band Structure of Spin-Orbit Coupled Materials", J.K. Desmarais, G. Ambrogio, G. Vignale, A. Erba, and S. Pittalis, Phys. Rev. Mater. 8, 013802 (2024)

[5] "Unveiling the Role of Spin Currents on the Giant Rashba Splitting in Single Layer WSe2", A. Boccuni, B. Peluzo, F. Bodo, G. Ambrogio, M. Jefferson, D. Mitoli, G. Vignale, S. Pittalis, E. Kraka, J. Desmarais, A. Erba, Phys. Chem. Lett. 15, 7442 (2024)

[6] "Electron localization function for non-collinear spins", J.K. Desmarais, G. Vignale, K. Bencheikh, A. Erba, S. Pittalis, https://arxiv.org/abs/2405.15530v2 [Accepted in Phys. Rev. Lett.]

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