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Field-induced exotic electronic phases in spin-filter tunnel junctions

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ABSTRACT:
The future of spintronics based on 2D-materials is dependent on the effectiveness of the injection of pure spin current into a tunnel barrier region. Here, first principles calculations are used to show that the efficiency of the spin-filtering across the semiconducting barriers of monolayer hBN is mainly limited by the dynamical response of tunneling electrons to the applied axial field. By projecting the effective electric field gradient densities and magnetic shielding constants across constitutive atomic layers in the scatter region of spin-filter tunnel junctions, an unusual site-dependent spin response is unraveled at the Fe/hBN and hBN/metal heterobilayer interfaces. Since the ground-state energy has no lower bound in extended electric fields, our analyses of the dependence of the Fermi surface topology on applied electric fields show the emergence of a frustrated electronic order. This exotic electronic phase is characterized by electric-field induced spin-flip relative to the ferromagnetic ground state, and observable as field-tunable perpendicular magnetic anisotropy.

HPC Content:
All the calculations were performed in parallel using version 6.4.1‘ of the Quantum ESPRESSO suite. Due to poor code scalability, all the computations were carried out on the ‘SMP que’ using 1 Node of 24 CPU cores. No net gain in computing speed was observed when more nodes were used on larger system sizes. In fact, the speed of the computations significantly reduced to > 6 CPU hours per scf-cycle when the same jobs were running on the ‘Normal que’ at 10 Nodes at double the system-size. The main computational challenge lies in solving the associated Poisson’s equation for atoms in the presence of the compensating potential due to externally-applied fields under gauge-corrections, in a more efficient manner. For fully-converged field-dependent computations, an average duration per task was timed at 2d 0h19m (CPU time) and 2d 0h40m (WALL time). This is still too ‘slow’ for scientific computing jobs executed on a supercomputer.

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