First-principles modelling of spin current in Co/NiCu spintronic terahertz emitters

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Spintronic terahertz emitters convert an ultrafast laser-driven spin current into a broadband THz transient via spin–orbit mediated spin-to-charge conversion. Here we model the spin-current generation in a Co/NiCu bilayer emitter by combining a thermodynamic diffusion formalism with the *ab initio* approach. Spin-polarized electronic configuration of a Co/NiCu supercell is obtained from density-functional theory calculations. The electronic structure for each spin chanel is then propagated separately through the semiclassical Boltzmann transport equation with BoltzTraP2 [1] to extract spin-dependent electrical conductivity and Seebeck coefficients. Spin current and its dependence on temperature gradients and channel asymmetry were further calculated with the phenomenological framework proposed by Fognini *et al.* [2]. The resulting workflow provides a first-principles route to quantify interfacial influence on the spin-current in bilayered metallic THz emitters.

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[2] Fognini A, Michlmayr T U, Vaterlaus A and Acremann Y 2017 *Journal of Physics: Condensed Matter* **29** 214002