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First-principles investigation of transient spin transfer torque in magnetic layers ZHIZHOU YU, JIAN WANG, The Univ of Hong Kong — By employing the nonequilibrium Green's function (NEGF) method, the transient current-induced spin transfer torque (STT) of the magnetic layered system is investigated based on the density functional theory (DFT). The computational cost of the transient STT is huge due to the dense mesh of k-sampling for the layered system. In order to speed up the calculation, the Hamiltonian of leads is replaced by the complex absorbing potential (CAP) so that the Green's function can be cast into the wide-band form. After employing the Padé spectrum decomposition, the energy integrals in the formalism of transient electric current and STT, including that of the Fermi distribution function, can be analytically calculated by the theorem of residue, which dramatically reduces the computational complexity of the transient STT. As an application, the NEGF-DFT-CAP formalism with the Padé approximation is implemented to study the transient electric current and current-induced STT of Co/Cu/Co trilayers under an upward pulse of bias with different rotating angles of magnetization direction between two leads. The oscillation behavior is obtained for the transient STT when it approaches the steady state.

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