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First-principles studies of the piezomagnetic effect in transition-metal fluorides SAI MU, KIRILL BELASHCHENKO, Univ of Nebraska - Lincoln — The piezomagnetic effect can facilitate the manipulation of magnetization by strain, especially in combination with a piezoelectric element. We formulate a model suitable for the first-principles evaluation of the piezomagnetic coefficients and apply it to the series of transition-metal fluorides (MnF_2, FeF_2, CoF_2). The longitudinal piezomagnetic tensor component Λ_{zxy} reaches a maximum at finite temperature similar to the longitudinal magnetoelectric susceptibility. This component is due to the symmetry-breaking response of the parameters of the microscopic spin Hamiltonian to strain, which is calculated from first principles. The transverse component Λ_{xyz}, which is entirely due to spin-orbit coupling, is evaluated by minimizing the total energy with respect to the canting of the local moments. The results are compared with available experimental data.

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