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$\mathbf{k}\cdot\mathbf{p}$ formalism within FLAPW method TATSUYA SHISHIDOU, TAMIO OGUCHI, Hiroshima University — We provide $\mathbf{k}\cdot\mathbf{p}$ formalism within the full-potential linearized augmented plane wave (FLAPW) method. Unlike the pure plane waves, the LAPW functions do not behave trivially in moving from $\mathbf{k}$ to $\mathbf{k}+\mathbf{q}$ and their incompleteness as a basis set should be taken into account. Derivatives of the sphere matching coefficients play the key role, for which we find a simple formula. Concrete formula for the $\mathbf{k}\cdot\mathbf{p}$ matrix elements is derived and numerically tested. Generalized second-order perturbation theory allowing for a degenerate case is presented and the literally-exact electronic band gradients and curvatures are accessible.

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