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First-Principles study of Hall coefficient in some cubic metals using Maximally localized Wannier functions

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Abstract
Calculation of Hall coefficient in semiclassical approach requires the first and the second derivatives of the energy bands at the Fermi level. We use the Maximally Localized Wannier Function technique to determine the required band derivatives and calculate the ordinary Hall conductivity and ordinary Hall coefficient in Al,Cu, Pd, Li, Au, Ag and Pb cubic metals.

Keywords: first-priniciple study, MLWF'S, Pb, Pd, Li, Cu, Au, Ag, Al, wave packet, Hall coefficient

For full article, refer to the Persian section