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Unfolding the Berry curvature of supercell calculations RAFFAELLO BIANCO, RAFFAELE RESTA, Univ Trieste, Italy, IVO SOUZA, Universidad del Pais Vasco, Spain — Unfolding band structures of supercell calculations has become a valuable tool for visualizing the influence of point impurities on the electronic states in crystals. In the same spirit, we introduce a procedure which maps the k-space Berry curvature of the occupied states from the small BZ of a supercell onto the normal BZ of the perfect (or virtual) crystal. As an application, we analyze the k-space distribution of the unfolded curvature of bcc $Fe_{1-x}Co_x$ ordered alloys, to better understand the influence of alloying on the anomalous Hall conductivity. Comparing with the ordinary curvature calculated in the virtual-crystal approximation, we find that the lowering of translational symmetry by the Co "impurities" introduces "extrinsic" contributions, which correlate with changes in the spectral function near the Fermi surface. In particular, the unfolded curvature displays additional sharp peaks associated with low-energy *pseudovertical* transitions. These occur in regions of k-space where two unfolded bands, which in the virtual crystal would be separated in k-space (and therefore would not jointly contribute to its Berry curvature), lie on either side of the Fermi level and are coupled by the impurity potential.

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