Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Weyl nodes in the bandstructure of bcc iron IVO SOUZA, Universidad del Pais Vasco, DAVID VANDERBILT, Rutgers University — Weyl points in 3D bandstructures are receiving increasing attention in connection with topological states of matter. In addition, a controversial suggestion has recently appeared[1] to the effect that isolated touching points between fully occupied and partially occupied bands, which act as monopole sources of Berry curvature, give a non-quantized, non-Fermi-surface contribution to the intrinsic anomalous Hall conductivity of ferromagnets. With these motivations, we carry out a systematic search for Weyl nodes in the bandstructure of bcc Fe using first-principles calculations. We trace the evolution of the Chern index of the fully occupied 2D bands in the (k_x, k_y) plane as a function of k_z, and find several touching events taking place at high-symmetry points and lines in the 2D BZ. The amount of Chern-number transfer is analyzed in terms of the symmetry labels of the crossing bands.[2] In addition to conical intersections with a topological charge $q = 1$, we find quadratic touching points with $q = 2$ that are protected by C_4^z symmetry, as well as lines of degeneracy carrying a net topological charge.

[1]Y. Chen *et al.*, Phys. Rev. B **88**, 125110 (2013).
[2]C. Fang *et al.*, Phys. Rev. Lett. **108**, 266802 (2012).

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Date submitted: 11 Nov 2013 Electronic form version 1.4