

## Fine structures in electronic structure calculations

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Fine structure in the electronic structure at the Fermi level  $E_F$  can give rise to unusual behavior. A recent example is provided by  $\text{NbFe}_2$ , where a highly unusual  $(\delta k)^3$  wiggle near  $E_F$  correlates perfectly with the small doping level at which a quantum phase transition occurs, accompanied by non-Fermi liquid behavior in the vicinity at low temperature. Another example is the the fine structure in the electronic spectrum of the recently reported nickel carbide superconductor, body-centered tetragonal  $I4/mmm$   $\text{Th}_2\text{NiC}_2$  with  $T_c = 8$  K. The filled Ni  $3d$  band complex is hybridized with C  $2p$  and Th character to and through the Fermi level, and a sharply structured density of states arises only when spin-orbit coupling is included, which splits a zone-center degeneracy leaving a very flat band portion centered at the Fermi level. The flat part of the band corresponds to an effective mass  $m_z^* \rightarrow \infty$  with very large and negative  $m_x^* = m_y^*$ . Although the region over which the effective mass characterization applies is less than 1% of the zone volume, it yet supplies of the order of half the states at the Fermi level.

- [1] A J S Machado et al 2012 Supercond. Sci. Technol. 25 045010