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Does nesting really cause Charge Density Waves? MICHELLE JOHANNES, IGOR MAZIN, Naval Research Laboratory, Washington, D.C. — The concept of a CDW induced by Fermi-surface nesting originated from the Peierls idea of electronic instabilities in purely 1D metals and is now often applied to charge ordering in real, low-dimensional materials. The idea is that if Fermi surface contours coincide when shifted along the observed CDW wave vector, then the CDW is considered to be nesting-derived. We argue that only a tiny fraction, if any, of the observed charge ordering phase transitions are true analogues of the Peierls instability, *i.e.* that (a) there is substantial nesting of the FS, as quantified by a peak in Im $\chi_0(\mathbf{q})$ at the CDW wave vector; (b) this peak translates (as in the 1D case) into a peak in Re$\chi_0(\mathbf{q})$ at the same wave vector; (c) a divergence in the full electronic susceptibility causes the electronic subsystem to be unstable *without* ion shifts; and (d) *all* phonons are softened at the CDW vector. Using prototypical CDW materials $NbSe_2$, $NbSe_3$, and $CeTe_3$, we show that these conditions are hardly ever fulfilled, and that the CDW phases are actually structural phase transitions, driven by ionic rather than electronic instabilities. We also show mathematically that the original Peierls construction is so fragile as to be unlikely to apply to any real material.

Michelle Johannes

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