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Fermi surface nesting and the origin of the charge density wave in NbSe2 CHRISTOPHER HOWELLS, MICHELLE JOHANNES, IGOR MAZIN, Naval Research Laboratory — The origin of a charge density wave (CDW) transition in $NbSe_2$ and related transition metal dichalcogenides has been studied and hypothesized about for the past four decades. The idea that CDW formation is the result of Fermi surface nesting was put forward as early as 1978 and continues to be suggested in current papers. Using highly accurate density functional calculations, we make a detailed study of the band structure and Fermi surfaces of equilibrium and pressurized $NbSe_2$. We calculate the real part of the non-interacting susceptibility, $\Re\chi_0(\mathbf{q})$, which is the relevant quantity for a CDW instability and the imaginary part,$\Im\chi_0(\mathbf{q})$, which directly shows Fermi surface (FS) nesting. We show that there are very weak peaks in $\Re\chi_0(\mathbf{q})$ near the CDW wave vector, but that no such peaks are visible in $\Im\chi_0(\mathbf{q})$, definitively eliminating FS nesting as a factor in CDW formation. We discuss the effects of pressure and provide calculated de Haas van Alphen frequencies and effective masses that can be compared to experiment.

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