

# Supporting Information

Feng et al. 10.1073/pnas.1217292110

## SI Text

### Band Structure Calculation of the Fermi Surface

Band structure calculations were performed using the WIEN2K package with GGA (nonmagnetic) and GGA+U (antiferromagnetic) approximations in the full-potential linearized-augmented-plane-wave method (ref. 1 and references therein), where U is the Hubbard correlation term. Fig. S1 shows the Fermi surface from the nonmagnetic calculation, which is of course only an approximation of the paramagnetic phase in GdSi, because the local moment on Gd is set to zero. Despite including the spin-orbit interaction effects in the nonmagnetic calculation, the spin-orbit splitting of the Gd 4f electrons is much smaller than the experi-

mental value and there is a density-of-states contribution from Gd 4f electrons at the Fermi level. However, the third band in Fig. S1 is predominantly formed from Si states, which are strongly dispersing. We also have performed calculations in a model antiferromagnetic state, shown in Fig. S2. In the antiferromagnet, the Gd 4f states have saturated local moments, and there are no 4f states near the Fermi surface, because in the antiferromagnetic calculation of GdSi we can introduce a Hubbard U-correlation term to locate the Gd 4f states at the experimentally observed energy. Because the nesting wave vector is not at the commensurate wave vector, this leaves a sheet of Fermi surface following the reconstruction and displaces the density-of-states minimum in Fig. 5 of the paper slightly away from the Fermi energy.

1. Blaha P, Schwarz K, Madsen GKH, Kvasnicka D, Luitz J (2001) *WIEN2K, An Augmented Plane Wave Plus Local Orbitals Program for Calculating Crystal Properties* (Technische Universität Wien, Vienna, Austria).

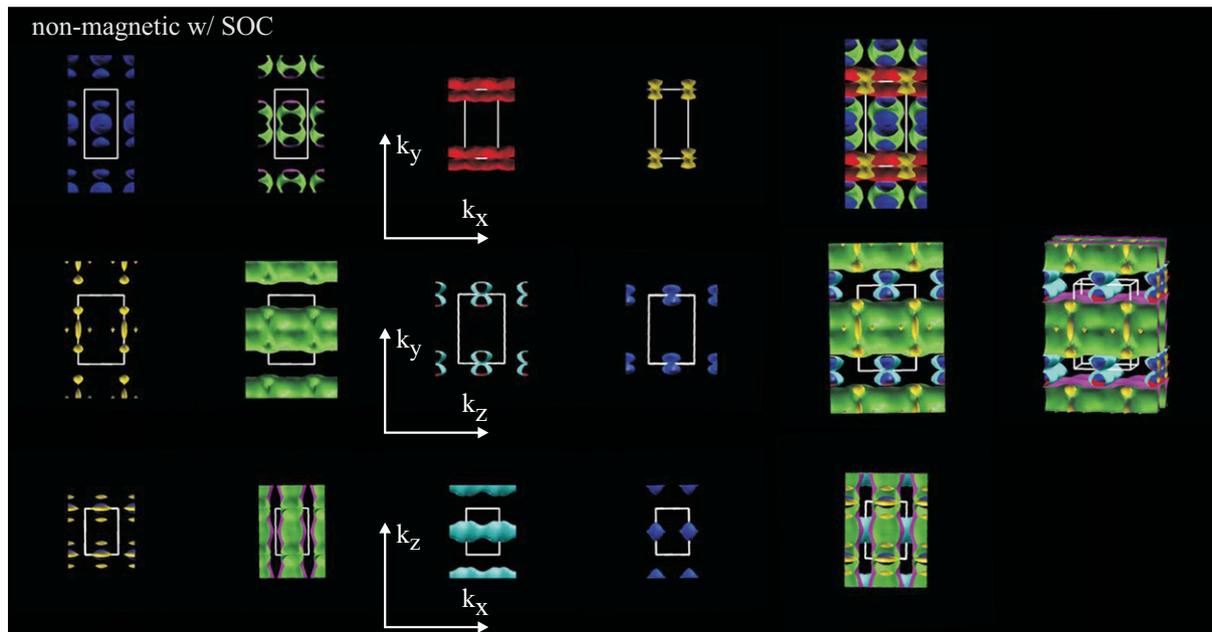


Fig. S1. Fermi surfaces from a nonmagnetic GGA approximation of the paramagnetic phase in GdSi.

