Electronic structure beyond the generalized gradient approximation for Ni_2MnGa

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I. FERMI SURFACE

Fig. S1 shows the Fermi surface for spin-up electrons calculated in the LSDA, GGA, and SCAN functionals. It is seen, the Fermi surface of the spin-up bands does not change significantly, band 31 (red) expands mainly.

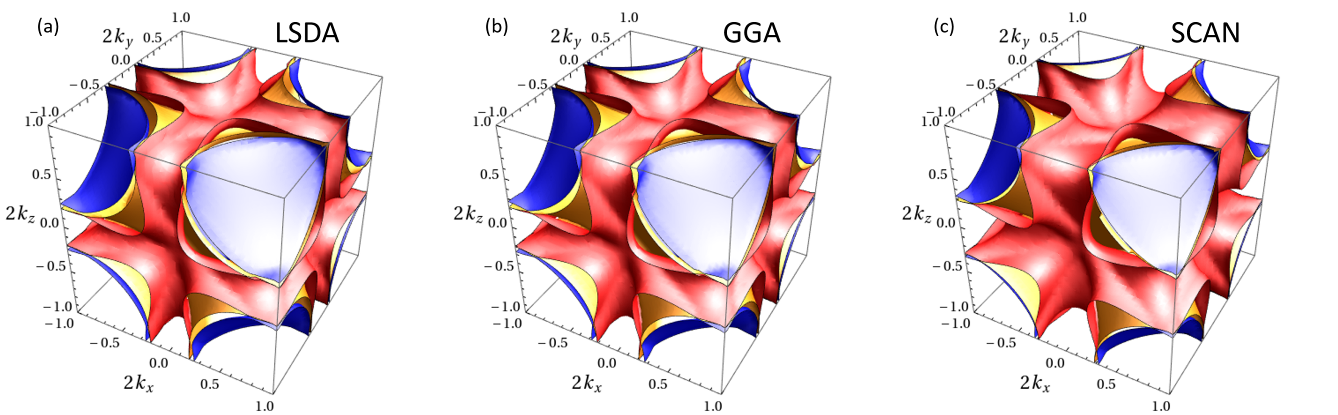

FIG. 1. Fermi surface for spin-up electrons for an austenitic structure of Ni_2MnGa.

II. GENERALIZED ELECTRONIC SUSCEPTIBILITY

Figure S2 shows the 2D-maps of $\chi(\mathbf{q})$ for the (110) plane calculated with LSDA, GGA, and SCAN. The curves for LSDA and GGA show two peaks, which are mainly due to the nesting of the spin-down channel. According to the 2D-maps, the results look similar for the minority contributions calculated with LSDA and GGA, while the majority contribution demonstrates some additional peaks of $\chi(\mathbf{q})$ in case pf GGA. SCAN considerable alters the 2D-map. In contrast to LSDA and GGA, there is no peak in the major channel for SCAN. Also, for the total contribution, two additional peaks are observed along the [110] direction.

III. SCAN$-U$

SCAN gives an overestimated magnetic moment [1–3]. To reduce it, we use SCAN$-U$. The influence of the parameter U on the Fermi surface is illustrated in Fig. S3. When U increases, the piece of band 64 indicated by orange expands, while the piece of band 63 indicated by blue becomes narrower. This trend leads to an increase in the length of the nesting vector.

To determine precisely the nesting vector, the generalized susceptibility curves are calculated with different approximations. The results for SCAN$-U$ ($U = 0.6$ and $U = 1.8$ eV) are presented in Fig. S4. In case of $U = 0.6$ eV, the $\chi(\mathbf{q})$ for spin-up bands does not show peaks and nesting. In contrast, $\chi(\mathbf{q})$ of spin-down bands shows two pronounced

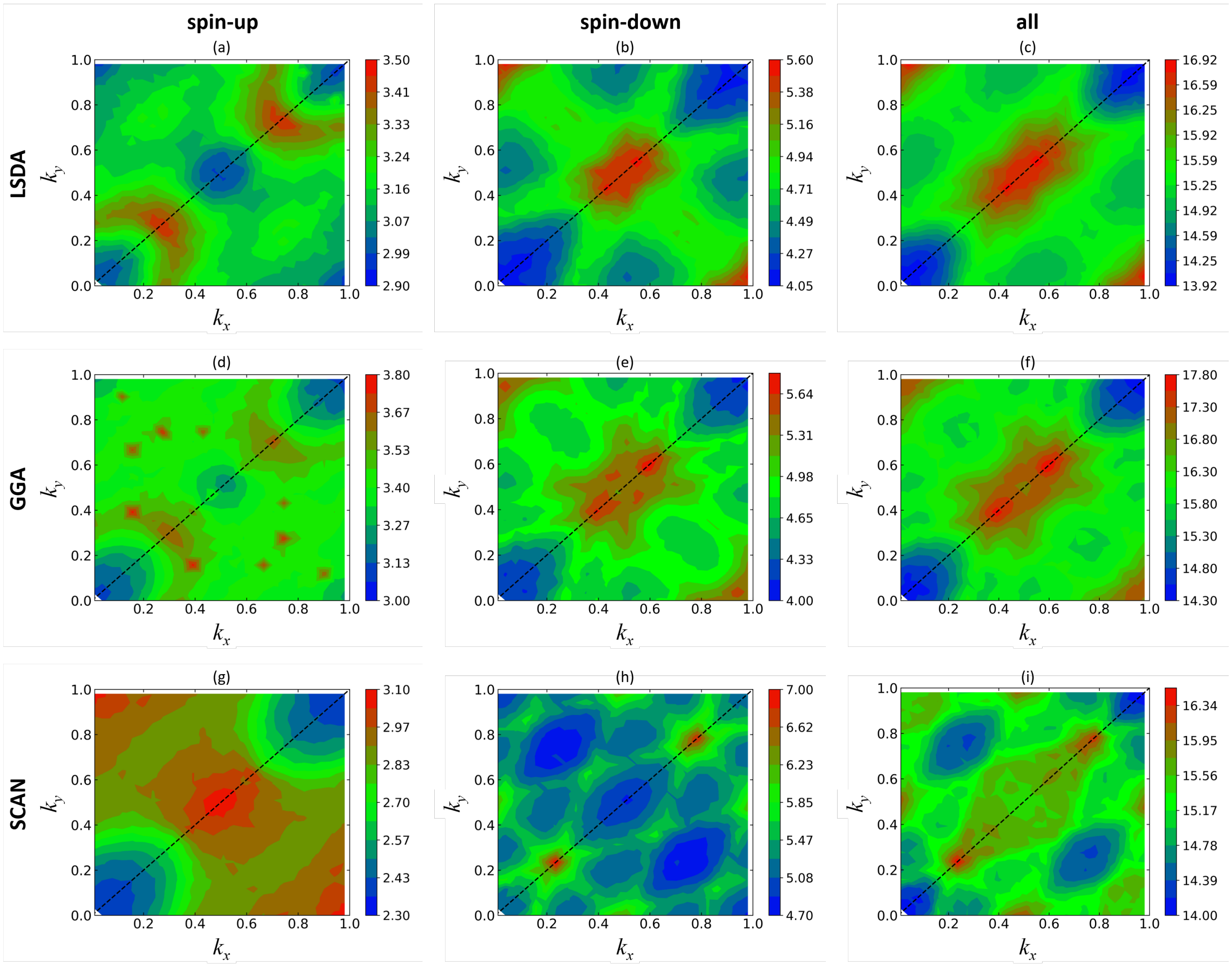

FIG. 2. Generalized susceptibility $\chi(\mathbf{q})$ for Ni_2MnGa. The top, middle, and bottom panels correspond to LSDA, GGA, and SCAN, respectively. The first, second, and third columns correspond to minority, majority, and total band contributions, respectively.

maxima, and the distance between them is slightly lower than in case of SCAN (see Fig. S2(c)). For total contribution, $\chi(\mathbf{q})$ displays four maxima for SCAN. However, for $U = 1.8$ eV, the profile of $\chi(\mathbf{q})$ becomes similar to GGA.

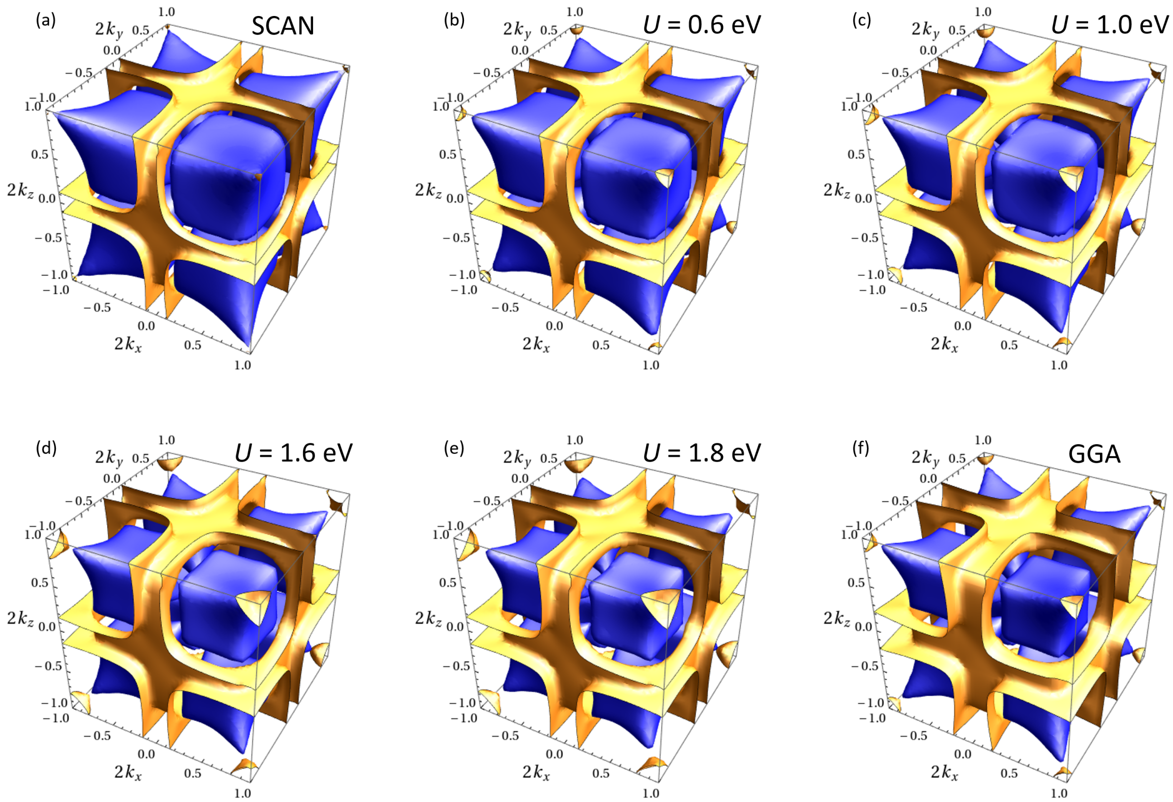

FIG. 3. Fermi surfaces calculated with SCAN, SCAN$-U$, and GGA for austenitic phase of Ni_2MnGa.

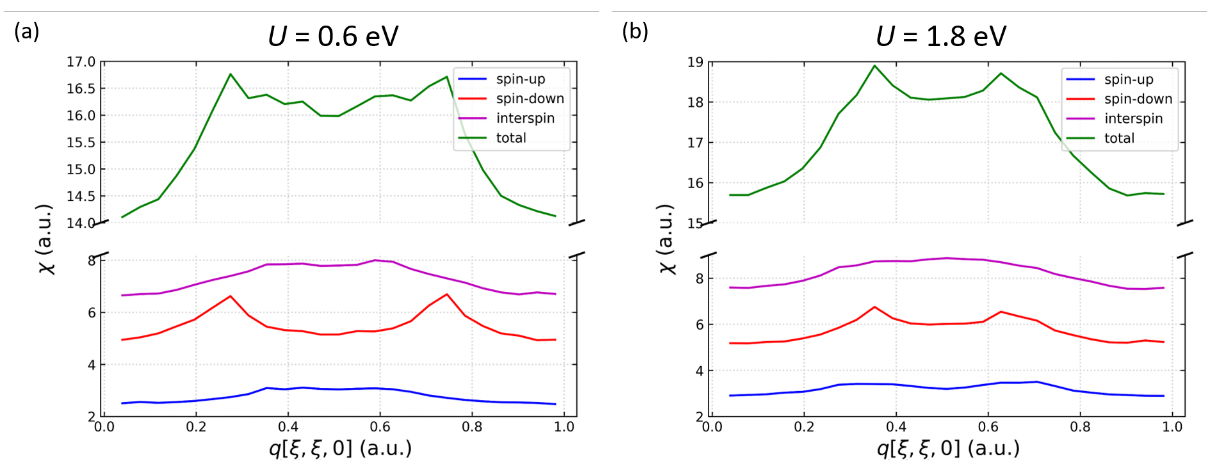

FIG. 4. Generalized susceptibility along the [110] direction calculated with SCAN$-U$ for $U = 0.6$ and 1.8 eV. The results are presented for spin-up, spin-down, interspin, and total contributions. Spin-up and spin-down are interspin contributions. The total contribution involves both intraspin and interspin contributions in the susceptibility calculation.

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