Electronic structure beyond the generalized gradient approximation for Ni$_2$MnGa

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The stability of the nonmodulated martensitic phase, the austenite Fermi surface, and the phonon dispersion relations for ferromagnetic Ni$_2$MnGa are studied using density functional theory. Exchange-correlation effects are considered with various degrees of precision, starting from the simplest local spin density approximation (LSDA), then adding corrections within the generalized gradient approximation (GGA), and finally, including the meta-GGA corrections within the strongly constrained and appropriately normed (SCAN) functional. We discuss a simple procedure to reduce a possible overestimation of magnetization and underestimation of nesting vector in SCAN by parametrically decreasing self-interaction corrections.

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I. INTRODUCTION

During the last decades, the intermetallic Heusler alloys family has attracted enormous interest because of a wide spectrum of the remarkable properties related to elasticity, magnetism, and thermodynamics [1–8]. In particular, ternary Heusler compounds with generic formula X$_2$YZ crystallize in L2$_1$-cubic structure in the austenite phase and can undergo a martensitic phase transition (MT) to lower symmetry structure upon cooling. In general, X and Y are 3d transition metals and Z is an sp element of III-V group in the periodic table. Usually, the martensitic temperature ($T_M$) depends on the chemical composition and thus on local interactions, plastic deformation, and heat treatment protocols [1,2,5]. For most compounds, $T_M < T_C$, where $T_C$ is the Curie temperature. As a result, the magnetic degrees of freedom are expected to strongly couple with the lattice, especially when $T_M$ is close to $T_C$ [1,9–11].

In 1996, Ullakko and collaborators studied the magnetic control over the shape-memory effect in the ferromagnetic Ni$_2$MnGa Heusler alloy [12]. These authors were able to induce reversible deformations of 0.2% by application of magnetic fields below 1 T. In 2002, a larger effect of about 10% was obtained in similar compounds with a slightly different composition [13]. Today, a great effort is deployed to search new Heusler compounds with optimal properties for sensors and actuators [2,14,15].

Concerning the origin of the MT in Ni$_2$MnGa [16], a theoretical explanation based on the Jahn-Teller effect has been proposed by Fuji et al. [17] from the calculated densities of states (DOS), which is also consistent both with another density functional theory (DFT) calculation by Ayuela et al. [18] and photoemission experiments by Opeil et al. [19]. However, the existence of three-layered premartensitic (3M), martensitic five-layered (5M), and seven-layered (7M) modulated phases in addition to the nonmodulated tetragonal phase cannot be explained by the Jahn-Teller effect only. As suggested by several authors (see, e.g., Refs. [20–23]), the formation of modulated phases is associated with an anomalous transverse acoustic TA$_2$ mode in the [110] direction at the wave vector $q = \frac{2\pi}{a} [\xi \xi 0]$ with $\xi \approx 0.33$ and, consequently, a softening of shear modulus $C'$. Thus, the parent cubic phase becomes unstable because the atomic planes can shuffle along the [110] direction and the premartensitic phase transition occurs at $T_P \approx 260$ K [24,25]. In the case of MT, the transition temperature is $T_M \approx 200$ K while the softening of TA$_2$ phonon branch is more pronounced [26], and it is shifted to $\xi \approx 0.43$. The role of the phonon anomaly in destabilizing the austenitic phase can be explained by the nesting of the austenitic Fermi surface (FS) [27] and the electron-phonon coupling [26,28]. The relationship between the premartensitic lattice softening with the generalized susceptibility singularities produced by the FS nesting has been reviewed by Katsnelson et al. [29].

For magnetic shape memory compounds, some important questions regarding this relationship remain to be clarified despite a large amount of work (for instance, see Refs. [4,19,26,27,30–33]) because of the lack of information on correlation effects present in martensitic ferromagnetic phases. Nevertheless, despite correlation effects, the FS nesting could still play an important role in the instability of the austenitic phase upon cooling. Velikokhatnyi and Naumov [30] have first explored the FS nesting by using DFT within local spin-density approximation (LSDA) [34,35] and concluded that the nesting vector parameter $\xi$ extracted from generalized susceptibility is approximately 0.42 justifying a
MT to the 5M phase rather than the premartensitic transition to the 3M phase. Lee et al. [31] with the same method observed a nesting vector in agreement with the experimental phonon anomaly [21,22] by renormalizing the value of the magnetic moment with the factor of 70%, which corresponds to the magnetization at \( T_\text{P} \).

Haynes et al. [27] conducted a comprehensive study combining positron annihilation experiments with linear muffin-tin orbital electronic structure calculations within LSDA [36]. These authors found that the peaks of the generalized susceptibility \( \chi(\mathbf{q}) \) appear both in spin-up and spin-down channels. Siewert et al. [32,33] examined the effect of corrections beyond LSDA on \( \chi(\mathbf{q}) \) in the framework of the generalized gradient approximation (GGA). Their results confirm that the FS nesting is present not only for spin-down channel but for spin-up as well. They also noticed new susceptibility peaks along other directions produced by GGA. Bungaro et al. [26] performed both phonon dispersion and FS calculations demonstrating that GGA corrections to LSDA are beneficial in order to improve the agreement between theory and experiment.

Since correlation effects in Ni$_2$MnGa appear to play a crucial role on total energies, DOS, and magnetic moments [37,38], we also expect major corrections beyond LSDA and GGA for describing FS nesting and phonon instabilities. A simple step forward is the strongly constrained and appropriate normed (SCAN) functional, which is the most promising meta-GGA scheme due to the number of exact constraints fulfilled by the exchange-correlation energy [39–41]. SCAN cures the unphysical interaction of an electron with itself, which occurs in LSDA and in GGA. The self-interaction correction (SIC) can be measured with a Coulomb energy \( U \), which is related to the exchange correlation hole [42]. It is possible for electrons at the Fermi surface, the SIC must be reduced [43] because of the itinerant character of the wave functions. The correction must in fact vanish in the limit of plane waves. To examine this possible SCAN overcorrection, we also consider a SCAN – \( U \) scheme, where the SIC is reduced by an amount \( U \) for the 3d orbitals on Mn atoms. This parametric study SCAN – \( U \) can provide a first understanding how to further improve SCAN for predicting functional Heusler alloys and their magnetic properties accurately.

The outline of the paper is as follows. Section II contains the computational methods and calculation details. Section III is devoted to the discussion of the results of exchange correlation corrections on FS, nesting vector, generalized susceptibility, and phonon dispersion relations. The concluding remarks are presented in Sec. IV.

II. CALCULATION DETAILS

The electronic structure calculations were performed using the spin-polarized DFT within the projected augmented wave (PAW) method implemented in Vienna ab initio simulation package (VASP) [44,45]. LSDA and GGA parametrized by Perdew-Zunger [46] and Perdew-Burke-Ernzerhof [47], respectively, were used to describe correlation energy. Effects beyond GGA are described with the meta-GGA corresponding to the SCAN implementation [41]. A parametric study was performed using SCAN – \( U \) method. The \( k \) points within the Brillouin zone were generated using a uniform Monkhorst-Pack [48] mesh of \( 12 \times 12 \times 12 \). The cutoff energy was set to 700 eV. The PAW pseudopotentials were generated with the following atomic configurations: Mn(3p$^6$3d$^5$4s$^1$), Ni(3p$^6$3d$^8$4s$^2$), and Ga(3d$^{10}$4s$^2$4p$^1$). The calculations were converged with the energy accuracy of \( 10^{-6} \) eV/atom. Conjugate gradient algorithm was used to minimize all the residual forces until the convergence criteria of 0.01 eV/Å.

For the FS modeling, the \( 51 \times 51 \times 51 \) Monkhorst-Pack \( k \) grid was used. The generalized susceptibility was calculated for both majority and minority spin channels as following [26,30,31]

\[
\chi(\mathbf{q}) = \sum_{n,m,k} \frac{f(\epsilon_m(\mathbf{k})) [1 - f(\epsilon_n(\mathbf{k}))]}{\epsilon_n(\mathbf{k} + \mathbf{q}) - \epsilon_m(\mathbf{k})},
\]

where \( f(\epsilon_{m(n)}) \) is the Fermi-Dirac distribution function and \( \epsilon_m(\mathbf{k}), \epsilon_n(\mathbf{k}) \) are energies corresponding to the \( m \) and \( n \) band at the wave vector \( \mathbf{k} \). The peaks of \( \chi(\mathbf{q}) \) indicate electronic instabilities associated with the FS nesting.

Phonon calculations along a single direction were performed using the PHONON [49,50] package. We used a 48-atom supercell consisting of three 16-atom initial tetragonal cells merged in the direction [110] of the tetragonal cell. The PHONON package uses Hellmann-Feynman forces obtained combined positron annihilation experiments with linear muffin-tin orbital electronic structure calculations within LSDA [36].

III. RESULTS AND DISCUSSIONS

The geometry optimization and ground state properties calculations were performed for cubic L2$_1$ (\( F\bar{m}m\bar{n}, \) No. 225) and tetragonal L1$_0$ (\( F\text{mmm}, \) No. 69) structures of Ni$_2$MnGa. Calculations were performed on four atoms cells both for austenitic and martensitic phases. For L2$_1$ structure, Ni atoms occupy \( 8c \) [(1/4, 1/4, 1/4) and 3/4, 3/4, 3/4] Wyckoff positions, while Mn and Ga atoms site at 4\( b \) (1/2, 1/2, 1/2) and 4\( a \) (0, 0, 0), correspondingly. For L1$_0$, Ni atoms site on 8\( f \) [(1/4, 1/4, 1/4) and 3/4, 3/4, 3/4] Wyckoff positions, Mn atom locates at 4\( b \) (0, 0, 1/2), and Ga atom sites at 4\( a \) (0, 0, 0). The results of geometry optimization for martensitic and austenitic structures obtained with LSDA, GGA, SCAN, and SCAN – \( U \) are presented in Table I.

A. Fermi surface and generalized susceptibility

Figure 1 shows the band structure in the vicinity of the Fermi level calculated at equilibrium volume of the austenitic phase. The Fermi level is crossed by bands as shown in Fig. 1(b). In this case, band 64 calculated within SCAN does not cross the Fermi level along the path K–\( \Gamma \) in contrast to LSDA and GGA indicating that some parts of the FS vanish.
TABLE I. The equilibrium lattice parameters \(a_0\) and \(a_t\) in Å, total magnetic moment \(\mu_{\text{tot}}\) in \(\mu_B/\text{f.u.}\), for austenitic and martensitic structure and energy difference between austenite and martensite \(\Delta E\) in meV/atom of Ni\(_2\)MnGa calculated with LSDA, GGA, SCAN, and SCAN – \(U\) (\(U = 1.0\) and 1.8 eV). For comparison, available experimental data are presented.

|          | Austenite | Martensite | \(\Delta E\) |
|----------|-----------|------------|--------------|
| LSDA     | 5.633     | 3.717      | 5.207 1.264 3.821 16.8 |
| GGA      | 5.807     | 4.105      | 5.384 1.250 4.137 8.1 |
| SCAN     | 5.726     | 4.726      | 5.378 1.213 4.667 11.9 |
| SCAN – \(U\) (\(U = 1.0\) eV) | 5.706 | 4.464 | 5.368 1.198 4.404 19.8 |
| SCAN – \(U\) (\(U = 1.8\) eV) | 5.690 | 4.173 | 5.308 1.230 4.081 28.1 |
| Expt.    | 5.825\textsuperscript{a} 3.63\textsuperscript{b} 5.52\textsuperscript{c} 1.18 \(\pm 0.02\textsuperscript{d}\) 4.23\textsuperscript{e} |

\(\textsuperscript{a}\)Ref. [16]  
\(\textsuperscript{b}\)Ref. [51] (at 230 K)  
\(\textsuperscript{c}\)Ref. [52]  
\(\textsuperscript{d}\)Ref. [53]  
\(\textsuperscript{e}\)Ref. [52]  
\(\textsuperscript{f}\)Ref. [51] (at 4.2 K)  

Figures 2(a)–2(c) show the minority spin FS for the austenitic phase within LSDA, GGA, and SCAN, which consists of two sheets corresponding to bands 63 and 64. The results for LSDA and GGA are in good agreement with previous studies [27,33]. As a consequence of the increased magnetic moment in SCAN, a remarkable modification of the minority FS occurs. In particular, the FS sheet associated to magnetic moment in SCAN, a remarkable modification of the structure and energy difference between austenite and martensite \(\Delta E\) in meV/atom of Ni\(_2\)MnGa calculated with LSDA, GGA, SCAN, and SCAN – \(U\) (\(U = 1.0\) and 1.8 eV). For comparison, available experimental data are presented.

The results for LSDA and GGA are in good agreement with previous studies [27,33]. As a consequence of the increased

\[ |q_1| = 0.43 \text{ and } 0.39 \text{ for LSDA and GGA, respectively.} \]

\[ |q_2| = 0.55 \text{ in LSDA and } 0.596 \text{ in GGA. The GGA results are in good agreement with the previous studies [30,31,33], SCAN alters considerably the form of the generalized electronic susceptibility in Fig. 3. This modification results in a significant separation of the two susceptibility peaks and the appearance of the additional peaks at |q_3| and |q_4| originating from interspin contribution. Moreover, according to the profile shown in Fig. 3, very different nesting vectors |q_1| and |q_2| are found. The values of their norms are |q_1| = 0.263 and |q_2| = 0.784. These results show that the correlation effects bring new singularities in \(\chi(q)\), which can explain a more complex landscape of the competing nonmodulated and modulated phases as in the case of stripes in cuprate superconductors [55]. Thus, SCAN modifies both spin-up and spin-down \(\chi(q)\) contributions.

B. Reduction of SIC

According to several authors [42,56], SCAN exaggerates the magnetic moment in some 3d transition metals [57,58]. The deorbitalization of the SCAN potential has been recently proposed to address this problem [56]. Another simple way to reduce SIC is to use a SCAN – \(U\) method, where \(U\) is a parameter measuring the excess of SIC. Figure 4 shows a parametric study of the SCAN SIC reduction. When \(U = 0\), we have full SIC, while a finite \(U\) measures the suppression of SIC.
As expected, the FS shape becomes more similar to the GGA case when a larger value of $U$ is removed from SCAN (see SM [54]). At the same time, the magnetic moment decreases and approaches the GGA value of $4.17 \mu_B$ in austenite when $U \approx 2$ eV. Concerning $\chi(q)$, the reduction of SIC leads to the merging of the peaks ($q_1, q_3$) and ($q_2, q_4$) when the critical value $U = 1$ eV is reached. In this case, the 2D map shown in SM [54] becomes similar to the GGA 2D map.
From this parametric study, we deduce that SIC associated with SCAN corresponds to an effective GGA + $U$ scheme with $U \approx 2$ eV. This value of $U$ is significantly lower than the one proposed by Himmetoglu et al. [38] ($U = 5.97$ eV) and the one proposed by Sağdoğu et al. [59] ($U \approx 4$ eV for Mn atom). One should keep in mind that within the GGA + $U$ method, increasing $U$ on Mn sites results in a stronger SIC for the 3$d$-Mn orbitals. Several authors [60–62] have shown that the parameter $U$ is needed to obtain better agreement with experiments for elastic constants, tetragonal ratios, and magnetic anisotropy energy of Ni$_2$MnGa. In particular, Refs. [61,62] have shown that $U$ should be 1.8 eV for Mn. This value is smaller than the effective Coulomb correlation of 2 eV in SCAN, therefore in order to improve the agreement with the experiment, one needs to consider a revised SCAN scheme where the SIC is reduced at the Mn sites. In our case, the use of $-U$ mimics this SIC reduction. SIC reductions for systems with partially filled 3$d$ bands has been discussed by Barbiellini and Bansil [42].

C. Phonons

In the case of the austenitic phase, Bungaro et al. [26] showed that GGA gives imaginary phonon frequencies at zero temperature. In SCAN, the appearance of the additional peaks in $\chi(q)$ makes this phase even more unstable. This can lead to softening of additional acoustical modes.

Figure 5 shows the phonon dispersion in the case of nonmodulated martensitic L1$_0$ phase. The GGA phonon dispersion yields real frequencies for all phonon wave vectors in agreement with the calculation by Zayak et al. [63]. The SCAN calculation reveals an unstable mode near the $\Gamma$ point as shown in Fig. 5. Such small instability could be due to the fact that the landscape of almost degenerate solutions within SCAN usually becomes very complex as shown by Zhang et al. [55] therefore SCAN calculations are much more difficult to relax to the ground-state structure compared to the GGA. Interestingly, Himmetoglu et al. [38] claim that the ground state is a modulated martensite. Moreover, even within GGA, Zelený et al. [64] indicated that the 4O martensitic structure is 2 meV/atom below nonmodulated martensite solution.
IV. CONCLUSION

The concept of heterogeneity is important to explain large magnetic shape memory effects [65] in Ni$_2$MnGa, where new phases inside samples are themselves a heterogeneous modulation of their parent phase [66]. These modulated phases [67] can be stabilized within advanced DFT approaches beyond GGA. Competing inhomogeneous orders are a central feature of correlated electron materials, including the high-temperature superconductors. For example, by using schemes beyond GGA in YBa$_2$Cu$_3$O$_7$ [55], a new landscape of solutions characterized by stripe orders with large magnetic moments on Cu atoms have been recently uncovered. Similarly, one has found that the energy minimization with the same DFT scheme beyond the GGA is controlled by large Mn local moments in elemental manganese [68]. These observations demonstrate that correlation effects enable a new generation of understanding of the large magnetic shape memory effect and how this property emerges through the interplay of spin, charge, and lattice degrees of freedom.

Our results indicate that SCAN behaves as an effective GGA + $U$ scheme with $U$ parameter of about 2 eV. This amount of SIC captured by SCAN modifies the nesting properties of the austenitic FS and thereby creates new singularities in the electron susceptibility $\chi(\mathbf{q})$ justifying a more complex phase diagram. Consequently, the nonmodulated martensitic phase becomes unstable within SCAN as demonstrated by the softening of some calculated phonon modes. Moreover, the total magnetic moment increases significantly as in other 3$d$ transition metals such as iron [58]. This magnetic enhancement has been considered exaggerated in the literature. Therefore, it is possible that SIC corresponding to $U = 1.8$ eV should be renormalized toward the critical value $U = 1$ eV, where $\chi(\mathbf{q})$ starts to develop new singularities due to correlation effects. From the present results, we conclude that the amount of SIC in Ni$_2$MnGa can be measured by an effective $U$ in the interval of 1–2 eV.

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[1] A. N. Vasil’ev, V. D. Buchel’nikov, T. Takagi, V. V. Khovailo, and E. I. Estrin, Phys. Usp. 46, 559 (2003).
[2] V. D. Buchel’nikov, A. N. Vasilev, V. Koledov, S. Taskaev, V. V. Khovaylo, and V. G. Shavrov, Phys. Usp. 49, 871 (2006).
[3] P. Entel, V. D. Buchelnikov, V. V. Khovailo, A. T. Zayak, W. A. Adeagbo, M. E. Gruner, H. C. Herper, and E. F. Wassermann, J. Phys. D Appl. Phys. 39, 865 (2006).
[4] P. Entel, V. D. Buchelnikov, M. E. Gruner, A. Hucht, V. V. Khovailo, S. K. Nayak, and A. T. Zayak, Mater. Sci. Forum 583, 21 (2008).
[5] A. Planes, L. Mañosa, and M. Acet, J. Phys. Condens. Mat. 21, 233201 (2009).
[6] P. Entel, M. E. Gruner, A. Dannenberg, M. Siewert, S. K. Nayak, H. C. Herper, and V. D. Buchelnikov, Mater. Sci. Forum 635, 3 (2010).
[7] P. Entel, A. Dannenberg, M. Siewert, H. C. Herper, M. E. Gruner, V. D. Buchelnikov, and V. A. Chernenko, Mater. Sci. Forum 684, 1 (2011).
[8] T. Hickel, M. Uijttewaal, A. Al-Zubi, B. Dutta, B. Grabowski, and J. Neugebauer, Adv. Eng. Mater. 14, 547 (2012).
[9] A. D. Bozhko, A. N. Vasil’ev, V. V. Khovailo, V. D. Buchel’nikov, I. E. Dikshtein, S. M. Seletskii, and V. G. Shavrov, JETP Lett. 67, 227 (1998).
[10] A. N. Vasil’ev, A. D. Bozhko, V. V. Khovailo, I. E. Dikshtein, V. G. Shavrov, V. D. Buchelnikov, Matsumoto, S. Suzuki, T. Takagi, and J. Tani, Phys. Rev. B 59, 1113 (1999).
[11] V. V. Khovaylo, V. D. Buchelnikov, R. Kainuma, V. V. Koledov, M. Ohtsuka, V. G. Shavrov, T. Takagi, S. V. Taskaev, and A. N. Vasilev, Phys. Rev. B 72, 224408 (2005).
[12] K. Ullakko, J. K. Huang, C. Kantner, R. C. O’Handley, and V. V. Kokorin, Appl. Phys. Lett. 69, 1966 (1996).
[13] A. Sozinov, A. A. Likhachev, N. Lanska, and K. Ullakko, Appl. Phys. Lett. 80, 1746 (2002).
[14] S. A. Wilson, R. P. Jourdain, Q. Zhang, R. A. Dorey, C. R. Bowen, M. Willander, Q. U. Wahab, M. Willander, S. M. Alhilli, O. Nur, E. Quandt, C. Johansson, E. Pagounis, M. Kohl, J. Matovic, B. Samel, W. van der Wijngaart, E. W. Jager, D. Carlsson, Z. Djimovic, M. Wegener, C. Moldovan, R. Iosub, E. Abad, M. Wendlandt, C. Rusu, and K. Persson, Mater. Sci. and Eng.: R: Reports 56, 1 (2007).
[15] A. Irzhak, V. Koledov, D. Zakharov, G. Lebedev, A. Mashirov, V. Afonina, K. Akatyeva, V. Kalashnikov, N. Sitnikov, N. Tabachkova, A. Shelyakov, and V. Shavrov, J. Alloy. Compd. 586, S464 (2014).

[16] P. J. Webster, K. R. A. Ziebeck, S. L. Town, and M. S. Peak, Philos. Mag. B 49, 295 (1984).

[17] S. Fujii, S. Ishida, and S. Asano, J. Phys. Soc. Jpn. 58, 3657 (1989).

[18] A. Ayuela, J. Enkovaara, K. Ullakko, and R. M. Nieminen, J. Phys.: Condens. Matt. 17, 2011 (1999).

[19] C. P. Opeil, B. Mihaila, R. K. Schulze, L. Mañosa, A. Planes, W. L. Hults, R. A. Fisher, P. S. Riseborough, P. B. Littlewood, J. L. Smith, and J. C. Lashley, Phys. Rev. Lett. 100, 165703 (2008).

[20] A. Vasil’ev, V. Kokorin, Y. I. Savchenko, and V. Chernenko, Sov. Phys. JETP 71, 803 (1990).

[21] A. Zheludev, S. M. Shapiro, P. Wochner, A. Schwartz, M. Wall, and L. E. Tanner, Phys. Rev. B 51, 11310 (1995).

[22] A. Zheludev, S. M. Shapiro, P. Wochner, and L. E. Tanner, Phys. Rev. B 54, 15045 (1996).

[23] V. A. Chernenko, V. V. Kokorin, A. N. Vasil’ev, and Y. I. Savchenko, Phase Transit. 43, 187 (1993).

[24] U. Stuhr, P. Vorderwisch, V. V. Kokorin, and P.-A. Lindgård, Phys. Rev. B 56, 14360 (1997).

[25] V. V. Khovailo, T. Takagi, A. D. Bozhko, Matsumoto, J. Tani, and V. G. Shavrov, J. Phys.: Condens. Matt. 13, 9655 (2001).

[26] C. Bungaro, K. M. Rabe, and A. D. Corso, Phys. Rev. B 68, 134104 (2003).

[27] T. D. Haynes, R. J. Watts, J. Laverock, Z. Major, M. A. Alam, J. Wan, X. Lei, S. Chen, and T. Hsu, Scr. Mater. 52, 123 (2005).

[28] I. O. Velikokhatnyi and I. I. Naumov, Phys. Solid State 41, 617 (1999).

[29] Y. Lee, J. Y. Rhee, and B. N. Harmon, Phys. Rev. B 66, 054424 (2002).

[30] M. Siewert, M. E. Gruner, A. Hucht, H. C. Herper, A. Dannenberg, A. Chakrabarti, N. Singh, R. Arróyave, and P. Entel, Adv. Eng. Mater. 14, 530 (2012).

[31] M. Siewert, Electronic, magnetic and thermodynamic properties of magnetic shape memory alloys from first principles, Ph.D. thesis, University of Duisburg-Essen, 2012.

[32] S. H. Vosko, L. Wilk, and M. Nusair, Can. J. Phys. 58, 1200 (1980).

[33] J. P. Perdew, Phys. Rev. B 33, 8822 (1986).

[34] B. Barbiellini, S. Dugdale, and T. Jarlborg, Comput. Mater. Sci. 28, 287 (2003).

[35] V. D. Buchelnikov, V. V. Sokolovskiy, O. N. Miroshkina, M. A. Zagrebin, J. Nokelainen, A. Pulvkinne, B. Barbiellini, and E. Lähteenkorva, Phys. Rev. B 99, 014426 (2019).

[36] B. Himmetoğlu, V. M. Katukuri, and M. Cococcioni, J. Phys.: Condens. Matt. 24, 185501 (2012).

[37] J. P. Perdew, S. Kurth, A. Zupan, and P. Blaha, Phys. Rev. Lett. 82, 2544 (1999).

[38] J. Tao, J. P. Perdew, V. N. Staroverov, and G. E. Scuseria, Phys. Rev. Lett. 91, 146401 (2003).