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Bandstructure meets many-body theory: the LDA + DMFT method

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Abstract

Ab initio calculation of the electronic properties of materials is a major challenge for solid-state theory. Whereas 40 years' experience has proven density-functional theory (DFT) in a suitable form, e.g. local approximation (LDA), to give a satisfactory description when electronic correlations are weak, materials with strongly correlated electrons, say d- or f-electrons, remain a challenge. Such materials often exhibit 'colossal' responses to small changes of external parameters such as pressure, temperature, and magnetic field, and are therefore most interesting for technical applications.

Encouraged by the success of dynamical mean-field theory (DMFT) in dealing with *model* Hamiltonians for strongly correlated electron systems, physicists from the bandstructure and many-body communities have joined forces and developed a combined LDA + DMFT method for treating materials with strongly correlated electrons *ab initio*. As a function of increasing Coulomb correlations, this new approach yields a weakly correlated metal, a strongly correlated metal, or a Mott insulator.

In this paper, we introduce the LDA + DMFT method by means of an example, LaMnO₃. Results for this material, including the 'colossal' magnetoresistance of doped manganites, are presented. We also discuss the advantages and disadvantages of the LDA + DMFT approach.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The challenges of solid-state theory are to qualitatively understand a material's properties and to calculate these, quantitatively and reliably. This task is particularly difficult if electronic correlations are as strong as they are in many materials containing transition and rare-earth elements. Here, the Coulomb interactions between the valence electrons in d- and f-orbitals can be strong. The reason for this difficulty is that the standard approach, the *local* density approximation (LDA) [1], for calculating a material's properties relies on the electronic correlations in jellium, a weakly correlated system. For more correlated materials, the electronic density is strongly varying and the assumption of a constant density for treating exchange and correlation is not warranted. That is, the exact functional of density-functional theory [1], which, if known,

would allow the treatment of correlated materials, is certainly *non-local*. Another difficulty is the construction of functionals beyond ground-state properties, e.g. for spectral properties.

In this situation, we have seen a break-through brought about by a new method, LDA + DMFT [2–4], which merges LDA with dynamical mean-field theory (DMFT) [5–7] to account for the electronic correlations. This approach has been developed in an effort by theoreticians from the bandstructure and the many-body communities to join two of the most successful approaches of their respective fields. So far, LDA + DMFT has been successfully employed to calculate spectral, transport, and thermodynamic properties of various transition-metal oxides, magnetic transition metals, and rare-earth metals such as Ce and Pu (see [3, 4] for reviews). Depending on the strength of the Coulomb interaction, LDA + DMFT gives a weakly correlated metal as in LDA, a strongly correlated metal, or an insulator as illustrated in figure 1.

³ Deceased.

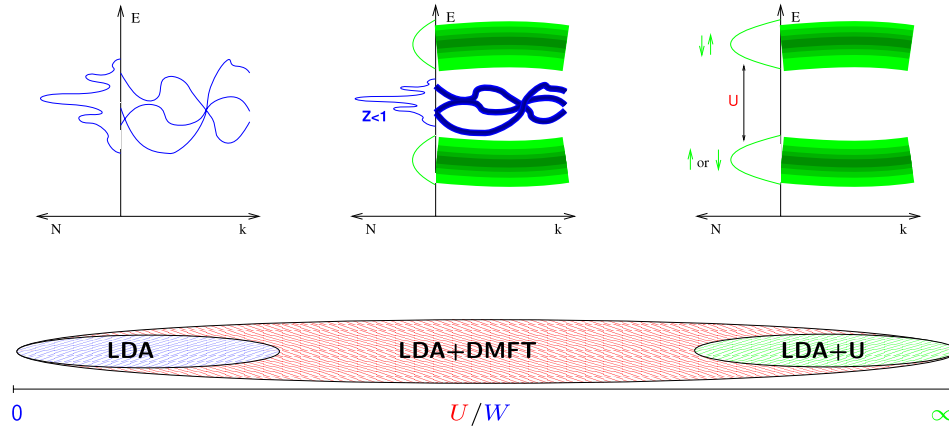


Figure 1. With increasing Coulomb interaction U (relative to the bandwidth W), we go from a weakly correlated metal via a strongly correlated metal with renormalized quasiparticles to a Mott insulator with a gap in the spectrum. The LDA bandstructure correctly describes the weakly correlated metal; LDA + U does so, with some restrictions [8], for the Mott insulator; and LDA + DMFT gives the correct physics in the entire parameter regime (reproduced from [4]).

In the following section, we will introduce this method with the example of a particular material currently of immense interest: the colossal-magnetoresistance (CMR) material LaMnO_3 . Results for the parent compound [9], as well as for doped manganites [10], are presented in section 3. Finally, in section 4, we conclude and discuss the pros and cons of LDA + DMFT.

2. LDA + DMFT in a nutshell

The first step in an LDA + DMFT calculation is the calculation of the LDA bandstructure. This paramagnetic bandstructure for our LaMnO_3 example is shown at the top of figure 2 for the ideal cubic structure. We employed the N th-order muffin-tin orbital (NMTO) basis set [11]. As we will later restrict the electronic correlations to the strongly interacting, more localized d- and f-orbitals, we need to identify these orbitals in the LDA calculation. In the case of LaMnO_3 where each Mn^{3+} ion is in the nearly cubic environment at the center of an oxygen octahedron, these are the three lower-lying t_{2g} and the two higher-lying e_g (3d) orbitals. Since Mn^{3+} has the d^4 configuration, the first three d-electrons occupy the t_{2g} orbitals forming a spin 3/2 according to Hund's rule. This leaves us with one electron per Mn in the two e_g orbitals. With a $t_{2g}^{\uparrow\uparrow\uparrow}e_g^{\uparrow}$ mean-field occupation (LSDA or LDA + U), only the e_g^{\uparrow} -like LDA bands would cross the Fermi level. For transition-metal oxides, one typically—in present day LDA + DMFT calculations—restricts the DMFT calculation to the low-energy bands crossing the Fermi level. Here, we employ NMTO downfolding [11] to obtain the effective LDA Hamiltonian for two Mn e_g orbitals, labeled $m = 1$ and 2 in figure 2. This Hamiltonian [10] can be written in terms of the 2×2 orbital matrix $\epsilon_{klm}^{\text{LDA}}$ whose diagonalization gives the LDA bandstructure (see first term of equation (1) given in figure 2). In other calculations, e.g. for Ce [12], all (spdf) valence orbitals have been taken into account. As shown in the top part of figure 2, the downfolded Hamiltonian (red bands) describes the LDA bandstructure of the LaMnO_3 e_g orbitals

very well. If other basis sets, such as plane waves, are used, the construction of a minimal set of well localized orbitals can be more involved. But this is also possible, for example, through Wannier-function projection [13, 14].

The second step of an LDA + DMFT calculation is to supplement the LDA Hamiltonian with the local Coulomb interaction which is responsible for the electronic correlations (see second part of figure 2). In general, the Coulomb interactions can be expressed, for example, by Racah parameters [15]. In actual calculations, however, this term has been hitherto restricted to the inter-orbital Coulomb interaction U' and Hund's exchange J (there is also a pair hopping term of the same size; see figure 2 top part, right-hand side). The intra-orbital Coulomb interaction $U = U' + 2J$ follows by symmetry. For a parameter-free (*ab initio*) calculation, the (screened) Coulomb interactions have to be determined. As LDA + DMFT calculations for a prototype transition-metal oxide, SrVO_3 [16], and a prototype rare-earth metal, Ce [12], showed, such *ab initio* LDA + DMFT calculations employing the constrained LDA [17] for determining U' and J work very well. There is some uncertainty of ~ 0.5 eV [18] in U' due to the ambiguity in defining the d-orbitals, leading to an additional error besides the LDA and DMFT approximations involved. This can be a problem if one is close to a transition and hence sensitive to small changes of U' , as is the case for V_2O_3 [19], for example, which is close to a Mott–Hubbard transition. But usually results do not alter dramatically upon changing U' by ~ 0.5 eV [18].

In the case of LaMnO_3 , the half-occupied t_{2g} orbitals prevent us from using standard constrained LDA calculations. Hence, we took the $U' = 3.5$ eV value from the literature [21] and $J = 0.75$ eV from the spin-up/spin-down splitting of a ferromagnetic LSDA calculation. In the following, the three t_{2g} electrons are taken into account as a (classical) spin-3/2, coupled through Hund's exchange \mathcal{J} to the e_g spin (see the second term of the Hamiltonian (1) in figure 2).

The third step of the LDA + DMFT calculation is to employ DMFT for solving the many-body Hamiltonian (1).

LDA+DMFT in a nutshell

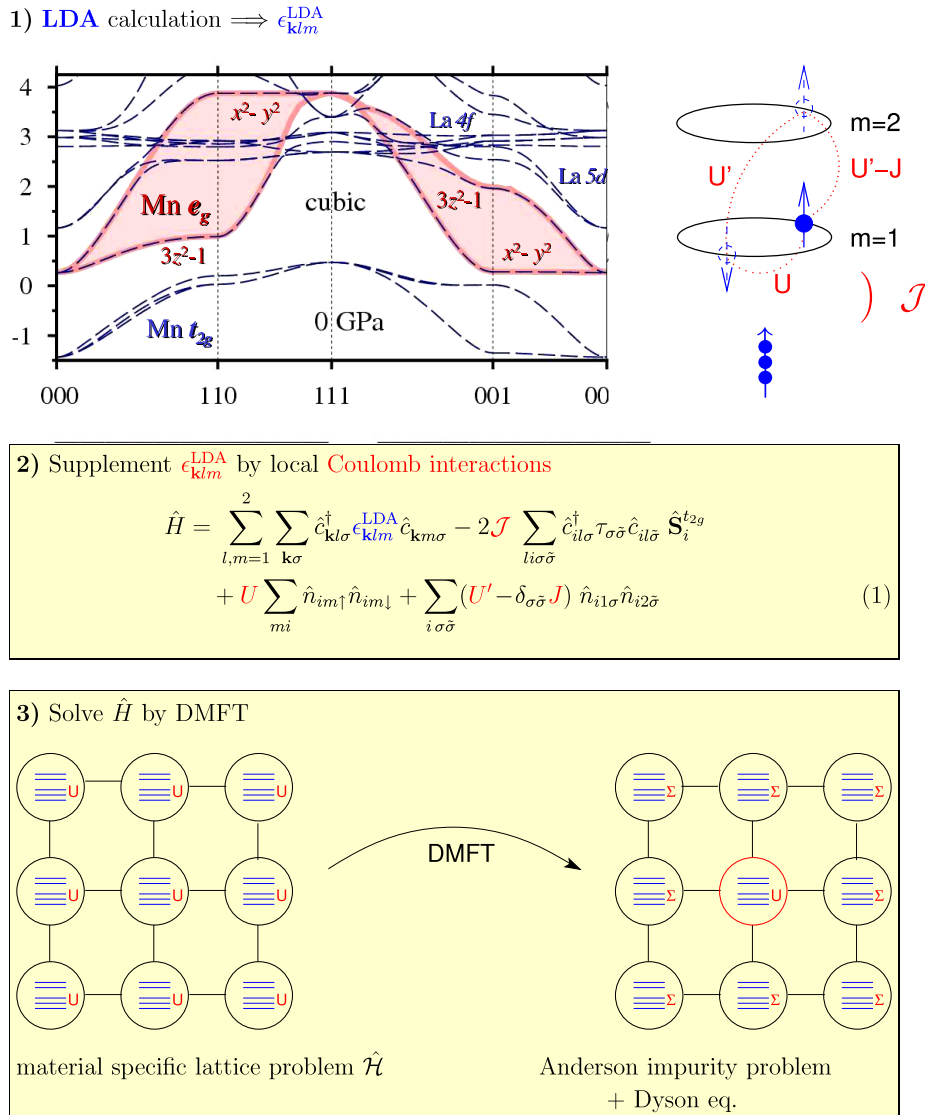


Figure 2. The three steps of an LDA + DMFT calculation.

Had we used the unrestricted Hartree–Fock (static mean-field) approximation instead, we would have the LDA + U approach [20]. In DMFT, we replace the Coulomb interaction at all sites, but one, by a self-energy. Electrons interact at this single site and still move through the whole lattice. However, at the other sites they propagate through the medium given by the self-energy instead of the interaction. This is the DMFT approximation, which hence neglects non-local vertex contributions. The emerging DMFT single-site problem is equivalent to an auxiliary Anderson impurity model [6] which has to be solved self-consistently together with the standard relation (Dyson equation) between self-energy and Green function. DMFT becomes exact [5] if the number of neighbors $Z \rightarrow \infty$ and is a good approximation for a three-dimensional system with many neighboring lattice sites. In particular, it provides for an accurate description of the major contribution of electronic correlation: the local correlations

between two d- or f-electrons on the same site. For more details on DMFT see [3, 4, 7].

If the electron density changes after the DMFT calculation, we have to go back to the first step and recalculate the LDA Hamiltonian for this new density. In contrast to the frequency-dependent spectral function, the electron density itself, however, only changes to a lesser degree. This self-consistency is therefore often left out.

An alternative point of view, besides the above-mentioned Hamiltonian one, is the spectral density-functional theory [22]. This theory states that the ground-state energy $E[\rho(\mathbf{r}), G_{ii}(\omega)]$ is a functional which depends not only on the electron density $\rho(\mathbf{r})$, but also on the local Green function (spectral function) $G_{ii}(\omega)$. LDA + DMFT is an approximation to this, in principle exact functional, in the same spirit as the LDA is to the exact density functional.

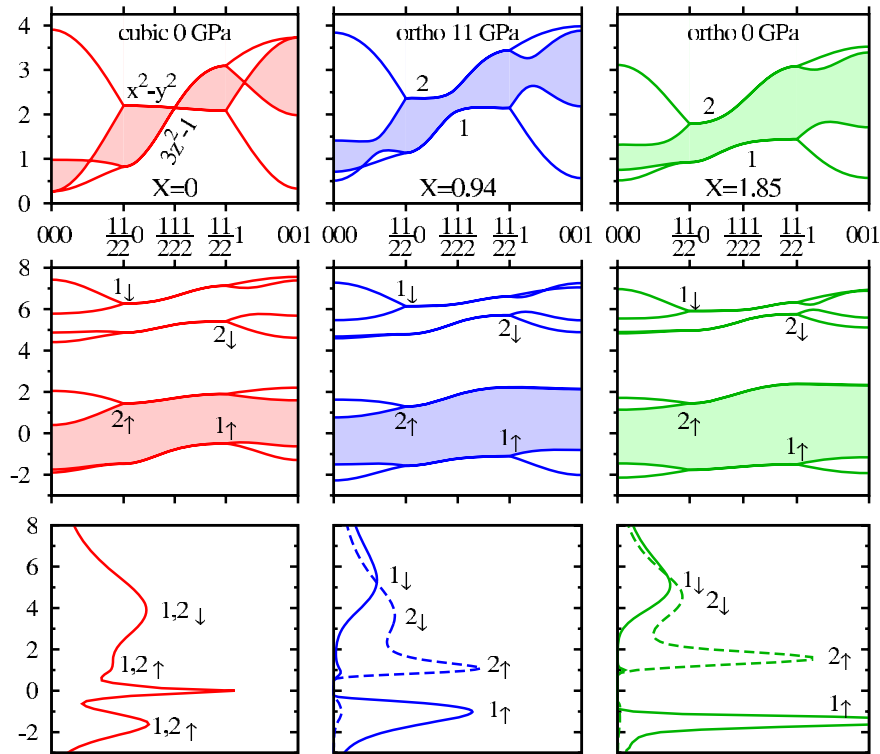


Figure 3. Bandstructure of paramagnetic LaMnO_3 as obtained in the LDA (top), LDA + U (center), and LDA + DMFT (bottom; k -integrated spectrum) for the experimental (orthorhombic) crystal structure at 0 GPa (right), 11 GPa (center) and an artificial cubic structure with the same volume as at 0 GPa (left). Energies are in eV with the Fermi energy being 0; the unit of k is π . For the correct insulating behavior and size of the gap, both Coulomb correlations and the crystal-field splitting due to the orthorhombic distortion are needed (bottom right). For more details see [9], from which this figure was reproduced.

3. Results for manganites

Let us now turn to the results obtained for LaMnO_3 . Figure 3 compares LDA, LDA + U and LDA + DMFT results for the real Jahn–Teller- and GdFeO_3 -distorted, orthorhombic crystal structure at 0 GPa and 11 GPa, as well as for an artificial cubic structure with the same volume as at 0 GPa. All LDA Hamiltonians were calculated for the paramagnetic phase, which is the stable one at 300 K. Even though the lattice distortion leads to a crystal-field splitting of the two e_g bands in the LDA, these bands still overlap. Hence, without electronic correlations, i.e. without U' , the plain vanilla LDA predicts a metal; it cannot describe the insulating paramagnet observed experimentally. If we now consider the many-body Hamiltonian (1) and treat it in the unrestricted Hartree–Fock approximation, we obtain the LDA + U bands shown in the middle panel of figure 3. We see that the crystal-field splitting becomes largely enhanced with the result that LaMnO_3 becomes an insulator, even in the cubic phase at compressions exceeding those for which the material is experimentally known to be metallic [23]. However, such effects are overestimated in the LDA + U approximation. We therefore turn to LDA + DMFT which does a better job in this respect. In the cubic phase, and even at normal pressure, LDA + DMFT yields metallic behavior. Hence, both Coulomb interaction and crystal-field splitting are necessary and work hand in hand to make LaMnO_3 insulating at normal pressure.

The resulting gap is slightly smaller than 2 eV as in experiment. Our LDA + DMFT calculations show that for LaMnO_3 to be metallic at pressures above the experimental 32 GPa, some distortion must persist. For further details see [9].

Most fascinating, both from the point of view of basic physics and of materials engineering, is the ‘colossal’ magnetoresistance [24] of doped manganites such as $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$. At low temperatures, doped manganites are bad-metallic ferromagnets, whereas at high temperatures they are insulating [25, 26] for a wide range of doping. Since Sr dopes holes in LaMnO_3 , one would generally expect a metallic behavior. As the lattice distortion fades away upon doping, we can start from a cubic crystal structure, for which the nearest-neighbor tight-binding hopping already gives an accurate description of the LDA bandstructure, as shown in [9]. Even without the static lattice distortion, we must, however, include the distortion in the form of phonons. We do so by the two Jahn–Teller phonons coupled to the e_g electrons through the electron–phonon coupling constant g .

These local Holstein phonons are described by a single frequency ω . Our DMFT calculation (see [10] for details) shows again that Coulomb interaction and electron–phonon coupling mutually support each other: On lattice sites with a single electron the Jahn–Teller coupling leads to a (dynamic) splitting of the two e_g levels which is strongly enhanced by the Coulomb interaction. In this way the electrons are localized as a lattice polaron, explaining the unusual experimental

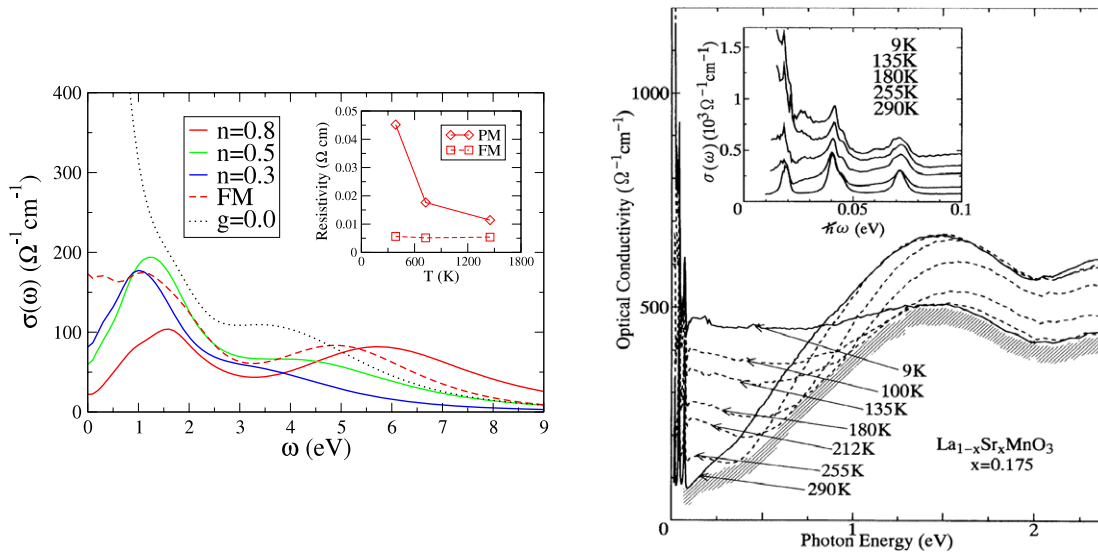


Figure 4. LDA + DMFT optical conductivity (left; reproduced from [10]) in comparison with experiment (right; reproduced from [26]) for the paramagnetic (PM) phase of $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ ($n = 1 - x$ electrons/site). The dotted line shows a metallic Drude peak in the absence of electron–phonon coupling; the dashed line the ‘bad’ metallic behavior in the ferromagnetic phase (FM) at $x = 0.2$. Inset: in the PM (FM) phase, the resistivity shows insulating (‘bad’ metallic) behavior so that the application of a magnetic field results in a ‘colossal’ magnetoresistance.

properties of doped manganites [27]. Figure 4 shows as an example the optical conductivity and the resistivity as a function of temperature. As one can see, the paramagnet has a (pseudo-)gap at low frequencies and is therefore insulating-like. In contrast the ferromagnet is a (bad) metal. Since the ferromagnetic phase can be stabilized by a small magnetic field, a ‘colossal’ magnetoresistance emerges.

4. Conclusion and perspectives

Using the example of LaMnO_3 , we introduced the LDA + DMFT approach and presented some of the results obtained. Let us conclude this paper by outlining the advantages and disadvantages of LDA + DMFT. The most striking advantages are:

- (i) We can now calculate the electronic properties of *strongly correlated 3d- and 4f-materials* with an accuracy comparable to that of the LDA for electronically weakly correlated materials.
- (ii) As the name *dynamical* mean-field theory suggests, the *dynamics* of the electrons is included, as are the excited states. One always calculates the excitation spectrum. These states are effective-mass renormalizations of the LDA one-particle states. Actually, we even have *two* effective-mass renormalizations of the LDA dispersion relation ϵ_k and a kink in between [28]. Also finite life times due to the electron–electron scattering and metal–insulator transitions are included.
- (iii) Besides the spectral function for the addition or removal of single electrons, correlation functions can also be calculated. From these two functions, all physical quantities can be calculated: spectra, transport properties, thermodynamics. All this naturally arises from a well-defined theory without the need to construct, for

example, from the LDA an effective Heisenberg model and from this, susceptibilities and critical temperatures (see, e.g., [29, 30] for such DMFT calculations)

With so many advantages, there are also disadvantages:

- (i) While the DMFT includes the major part of the electronic correlations, i.e. the *local* correlations induced by the local Coulomb interaction, non-local correlations are neglected. These give rise to additional, interesting physics, typically at lower temperatures, e.g. magnons, quantum criticality, and possibly high-temperature superconductivity. Recently, cluster [31] and diagrammatic extensions [32] of DMFT have been developed to overcome this obstacle.
- (ii) Another drawback is the computational cost for solving the Anderson impurity model. The numerical effort of the standard quantum Monte Carlo (QMC) simulations grows as $M^2(1/T)^3$ with a big prefactor for the Monte Carlo statistics. Here, M is the number of interacting orbitals. When n inequivalent ions with d- or f-orbitals are included in a supercell, the effort grows linearly $\sim n^1$. This means that typical LDA + DMFT calculations at room temperature require some hours on present day computers. The biggest problem is the $1/T^3$ increase of the computational effort. However, more recently developed QMC approaches, such as projective QMC [34] and continuous-time QMC [33], at least mitigate this drawback.
- (iii) At present the most important point preventing the widespread application of LDA + DMFT in academia and in industry is the lack of standardized program packages. But the inclusion of DMFT into well spread LDA codes, such as the Vienna *ab initio* simulation package (VASP) [35], for example, will certainly be done in the near future.

(iv) A more fundamental disadvantage is the need to identify the interacting d- or f-orbitals. This is cumbersome if one starts with plane waves and the result will also depend—to some extent—on the LDA basis set employed and the procedure for defining the d- or f-orbitals from these basis functions, e.g. via NMTO partial-wave downfolding or via Wannier-function projection.

With the pros clearly outweighing the cons, many of which have been or will be mitigated, LDA + DMFT or variants such as GW + DMFT will be used more and more in the future for calculations of correlated materials. With LDA and DMFT, bandstructure has finally met many-body theory. The next step is to meet industry.

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We would like to commemorate our young, dedicated co-worker, A Yamasaki, who prominently contributed to the original work presented in this paper.

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