Density functional theory calculations on magnetic properties of actinide compounds

Denis Gryaznov,ab Eugene Heifetsa and David Sedmidubskybc

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We have performed a detailed analysis of the magnetic (collinear and non-collinear) order and the atomic and electron structures of UO2, PuO2 and UN on the basis of density functional theory with the Hubbard electron correlation correction (DFT + U). We have shown that the 3-k magnetic structure of UO2 is the lowest in energy for the Hubbard parameter value of $U = 4.6$ eV (and $J = 0.5$ eV) consistent with experiments when Dudarev’s formalism is used. In contrast to UO2, UN and PuO2 show no trend for a distortion towards rhombohedral structure and, thus, no complex 3-k magnetic structure is to be anticipated in these materials.

1. Introduction

Actinide compounds continue to attract a great interest for both materials scientists and nuclear engineers. Their properties combine a strong electron correlation and relativistic effects of 5f valence electrons. In this paper, we study collinear and non-collinear magnetic structures of three basic actinide materials UO2, PuO2 and UN. All these materials have face-centred cubic (f.c.c.) actinide sub-lattice: the two oxides have fluorite structure and UN rock-salt structure. Experiments suggest that at low temperatures UN is anti-ferromagnetic1 with a collinear magnetic order, where U magnetic moments alternate along the (001) direction, while UO2 is anti-ferromagnetic (AFM) with the so-called noncollinear 3-k ordering of U magnetic moments (see Section 3 for more detailed description of different magnetic structures). The U magnetic moments in UN and UO2 in the AFM phases are very different, being 0.75 $\mu_B$ and 1.74 $\mu_B$, respectively. The Neél temperatures for both UO2 ($T_N = 30.8$ K, ref. 2) and UN ($T_N = 53$ K, ref. 1) are quite low. These two materials also differ in the chemical bonding. UN is evidently a conductor,3 whereas UO2 is a Mott insulator (as discussed, for example, in ref. 4). PuO2 is also a Mott insulator4 with magnetic susceptibility being temperature independent.5 All recent theoretical considerations6–9 employing the DFT + U technique or hybrid exchange-correlation functional (though without including spin–orbital interactions (SOI)) suggested the 1-k (collinear) AFM order for insulating PuO2, while experiment suggests that PuO2 is diamagnetic.

Thus, it is important to compare magnetic orders and accompanying lattice distortions for the considered compounds (UO2, UN, and PuO2) using the same method. Ignoring the lattice distortions may lead to a wrong electronic structure and significant errors in the defect energetics.10 As it was already mentioned, these materials reveal the same f.c.c. structure in the actinide sublattice. Therefore, similar structure of exchange interactions could be expected.

UO2 has been studied most intensively and now is much better understood in comparison with PuO2 and UN. UO2 is experimentally known to have a transverse 3-k magnetic structure and oxygen sub-lattice distortion of the same symmetry.11 To the best of our knowledge, the only first-principles modelling of the non-collinear magnetic ordering in UO2 was published by Laskowski et al.12 This study employed the DFT + U technique within the local spin density approximation (LSDA)13 and all-electron linearized augmented plane wave plus local orbitals method (L/APW + lo)14 as implemented in the Wien2k computer code. In these computations, the energetic preference of the 3-k structure with respect to a regular 1-k structure was primarily dependent on the method used to correct for a double counting of on-site interactions. The 3-k structure appears to be more stable, if the double counting correction accurately includes spin-polarization of the electron density,12 like it is done in LSDA + U15,16 or in a simplified rotationally-invariant approach by Dudarev et al.17 Nevertheless, the 1-k and 2-k magnetic structures were also suggested for UO2 prior to ref. 11. Also, no significant lattice distortions were found in these early experimental studies of UO2. Only recently, it was shown computationally19 for collinear AFM ordering in UO2 that the U magnetic moments alternate along the (111) direction, but not along the (001) direction, as it was generally assumed in nearly all previous computer simulations. For simplicity, we call these structures hereafter as the “(111) magnetic structure” and the “(001) magnetic structure”. The study19 based on the electronic structure calculations with hybrid exchange–correlation functional found that the rhombohedral unit cell has a lower energy than the tetragonal one, even though the SOI are not included. Thus, change from usual (001) magnetic structure to the (111) one could indicate possible non-collinear magnetism.

To the best of our knowledge, no such studies on the magnetic properties of PuO2 and UN have been performed so far. The X-ray diffraction measurements on UN revealed no significant tetragonal distortion,20 which would be a consequence of the AFM spin alignment along the (001) direction.

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a European Commission, Joint Research Centre, Institute for Transuranium Elements, Postfach 2340, Karlsruhe, D-76125, Germany. E-mail: EHefif5719@shcglobal.net
b Institute for Solid State Physics, University of Latvia, Kengaraga 8, LV-1063, Riga, Latvia. E-mail: gryaznov@mail.com
c Institute of Chemical Technology, Technicka 5, 16628 Prague, Czech Republic. E-mail: David.Sedmidubsky@vscht.cz

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In the present study, we consider possible collinear and non-collinear magnetic structures of UO$_2$ also using the DFT + U technique, but implemented in another code, Vienna Ab initio Simulation Package (VASP).\textsuperscript{21,22} First, we test the ability of this method and the code to reproduce experimentally observed non-collinear magnetic order in UO$_2$ using experimental values of the Hubbard parameter ($U = 4.6$ eV, $J = 0.5$ eV).\textsuperscript{24} Second, we explore different possible magnetic structures in UN and PuO$_2$ using the same DFT + U technique and try to determine which of the (001) and $\langle 111 \rangle$ structures is more stable. Section 2 describes computational details used in the present simulations. Descriptions of studied magnetic structures are given in Section 3. The results of our computations are provided and discussed in Section 4. Lastly, the conclusions are summarized in Section 5.

2. Computational details

In the present first-principles simulations we used the VASP (version 4.6)\textsuperscript{21,22} computer code employing the DFT + U method. The VASP code treats core electrons using pseudopotentials, whereas the semi-core electrons at U atoms and all the valence electrons are represented by plane waves. The electronic structure is calculated within the projector augmented wave (PAW) method.\textsuperscript{23} The simplified rotationally-invariant Dudarev’s form\textsuperscript{17} for the Hubbard correction was used for UO$_2$ and UN. It uses exclusively the difference, $U_{\text{eff}} = U - J$, of the Hubbard parameter $U$ and the exchange parameter $J$. In contrast to uranium compounds, PuO$_2$ shows a significant role of exchange part requiring the use of Liechtenstein’s form\textsuperscript{16} for the energy correction. The double counting correction in all our calculations was treated with account for spin-polarization.\textsuperscript{15–17} Computations of UO$_2$ were done including the SOI effects, whereas computations of PuO$_2$ and UN employed only scalar relativistic approximation. Both unit cell parameters and atomic positions were optimized until the energy convergence reached $10^{-5}$ eV. The calculations were performed with the cut-off energy of 520 eV. The integrations in the reciprocal space over the Brillouin zone (BZ) of the tetragonal unit cell of PuO$_2$ and UN (used to calculate the (001) AFM magnetic structure) were performed using $10 \times 10 \times 8$ and $12 \times 12 \times 10$ Monkhorst–Pack meshes,\textsuperscript{25} respectively. Computations of the rhombohedral PuO$_2$ and UN with the (111) magnetic structure were performed with $12 \times 12 \times 12$ and $14 \times 14 \times 14$ Monkhorst–Pack meshes. Similarly, the integrations over the BZ for the conventional unit cell of UO$_2$ were performed using $6 \times 6 \times 6$ Monkhorst–Pack meshes. The conventional 12-atom unit cell was necessary for modelling of UO$_2$ with non-collinear magnetic structures. It was possible to use the smaller unit cell for a collinear magnetic ordering (the 1-k AFM (001) and $\langle 111 \rangle$ magnetic structures) in UO$_2$. Correspondingly, in these cases we applied larger $14 \times 14 \times 10$ and $12 \times 12 \times 12$ k-meshes. The applied meshes in the reciprocal space were sufficient to reach a convergence of $10^{-4}$ eV for one-electron energies. Fractional electron occupancies were estimated with the Gaussian method using the smearing parameter of 0.25 eV. Calculations, which included SOI, were done with lifted symmetry constraints.

Photoemission spectroscopy (PS) measurements by Baer and Schoenes\textsuperscript{24} suggest that the Hubbard correlation parameter $U$ is 4.6 eV for UO$_2$ assuming that exchange parameter $J$ is 0.5 eV. These values were applied later by Dudarev \textit{et al.}\textsuperscript{17} In their calculations\textsuperscript{17} the band gap becomes open and equal to 1.3 eV within the LSDA + $U$, being, however, smaller than the experimental value of 2.0 eV. A somewhat better agreement is observed within the generalized gradient approximation,\textsuperscript{26} i.e. GGA + $U$.\textsuperscript{10,27–29} Note that following Dudarev’s calculations, we employed recently the same values of $U$ and $J$ in our study on bulk properties and defects behaviour in UO$_2$.\textsuperscript{10} In the present simulations we used the same set of correlation $U$ and exchange $J$ parameters for computations of UO$_2$. The parameter $U_{\text{eff}} = 1.875$ eV for UN was fitted\textsuperscript{20} to reproduce the magnetic moment of uranium ions and UN unit cell volume in the low-temperature phase. The band gap of $\sim 1.8$ eV\textsuperscript{31} for PuO$_2$ is known from the electrical conductivity measurements which is similar to the band gap in UO$_2$. Previous theoretical studies\textsuperscript{6–9} also agreed on the AFM solution for PuO$_2$ within the 1-k magnetism and, therefore, used the tetragonal structure as described above. Despite the relatively similar band gaps in both oxides, their electronic structures are quite different which is clearly seen in the corresponding PS measurements.\textsuperscript{32} Parameters $U = 3.0$ eV and $J = 1.5$ eV were fitted for PuO$_2$ to describe correctly its experimental lattice constant, band gap, and position of Pu 5f band.

3. Magnetic structures

The dependence of atomic magnetic moments on the position in a lattice can be expressed as expansion in plane waves:

$$M_j = \sum_{\nu=1}^{k} c_{\nu}^{\rho} (\hat{r}_j - \hat{r}_0) M_{\nu}^{\rho},$$

where $M_j$ is the magnetic moment of the atom in unit cell $j$ and at position $\hat{r}_j$, $\hat{r}_0$ is the position of the same atom in the 0th unit cell, $\hat{r}_w$ and $M_{\nu}^{\rho}$ are, respectively, the wave vector and amplitude of the magnetic wave $\nu$.

In the collinear 1-k magnetic structures magnetic moments of U atoms are collinear and changes in the magnetic moments can be described by a single wave ($k = 1$). For the (001) magnetic structure choosing the O$_z$ axis along the direction of alternation of magnetic moments, the wave vector is $k_1 = 2\pi/a$ (0, 0, 1), where $a$ is a cubic lattice constant. Similarly, for the (111) structure the wave vector is $k_1 = \pi/a$ (1, 1, 1). These two collinear 1-k magnetic structures were modelled for all three materials considered here. These magnetic structures have symmetry reduced from the cubic one. In the (001) structure the lattice has a tetragonal symmetry, and in the (111) structure the lattice becomes rhombohedral, as can be seen from the next section.

Farber \textit{et al.}\textsuperscript{18} suggested the 2-k transverse magnetic structure for UO$_2$ which is associated with a transverse phonon. If we choose the direction of the phonon propagation as the O$_x$ axis, then magnetic waves propagate along the O$_x$ and O$_z$ axes ($k_1 = 2\pi/a$ (1, 0, 0), $k_2 = 2\pi/a$ (0, 0, 1)) with amplitudes $M_{\nu}^{0} = M_0 (0, 1, 0), M_{\nu}^{1} = M_0 (1, 0, 0)$, where $M_0$ is...
the magnitude of atomic magnetic moment. Magnetic moments of U atoms lie on the Oxy plane and point along various [110] directions. The transverse phonon in this structure can be described as O atoms in odd and even (010) oxygen planes shift in opposite directions along the Ox axis. While later experiments showed that this structure is not the most stable one, we included it into our simulations to compare energies of all previously considered magnetic structures of UO₂.

According to the experiment,¹¹ UO₂ has transverse 3-k magnetic structure. The wave vectors for three waves in 3-k structures are \( k_1 = 2\pi/a (1, 0, 0), k_2 = 2\pi/a (0, 1, 0), \) and \( k_3 = 2\pi/a (0, 0, 1) \). There are two equivalent transverse structures with this symmetry in the fluorite lattice. The first structure has amplitudes \( M_0 = M_0 (1, 0, 0), M_y = M_0 (0, 0, 1), M_z = M_0 (1, 0, 0) \). The second one has amplitudes \( M_0 = M_0 (0, 0, 1), M_y = M_0 (1, 0, 0), M_z = M_0 (0, 0, 1) \). The two O atoms nearest to each U atom in the direction of its magnetic moment shift from their sites toward this U atom. Both structures have the same total energies. We used the first one in our simulations.

### 4. Results and discussion

In the present study, we assess the difference between the two (111) and (001) AFM magnetic collinear structures, as a function of the \( U \) and \( J \) parameters for UN and PuO₂ (Fig. 1).

The energy difference between the two magnetic structures for UN (Fig. 1a) is very small and negative at small values of \( U_{\text{eff}} = U - J \). It slowly grows for \( U_{\text{eff}} \) between 0.0 eV and 1.5 eV, then noticeably increases from 2.0 to 5 eV, and likely saturates for the higher values of \( U_{\text{eff}} \). For the optimized value of \( U_{\text{eff}} = 1.875 \text{ eV} \) the (001) structure of UN is already more stable than the (111) structure (see inset in Fig. 1a). At this value of \( U_{\text{eff}} \) the lattice constants for UN in the (001) magnetic structure are \( a = 4.974 \text{ Å} \) and \( c = 4.859 \text{ Å} \), and lattice parameters in the (111) magnetic structure are the lattice constant \( a = 4.942 \text{ Å} \) and the rhombohedral angle \( \gamma = 88.2^\circ \). In both cases the cubic unit cell is distorted along the direction of alternation of magnetic moments. In the (001) structure it is compressed along the Oz axis, for the (111) structure the unit cell is elongated along [111] direction. It is experimentally known that UN is cubic with the lattice constant \( a = 4.886 \text{ Å} \).³³ The calculated spin magnetic moments of U atoms are 1.47 \( \mu_B \) in the (001) structure and 1.82 \( \mu_B \) in the (111) structure. The magnetic moment of U atoms measured at low temperatures is 0.75 \( \mu_B \). Inclusion of the SOI allows revealing substantial orbital moments in actinide compounds which would lead to much better alignment of U atom magnetic moment with experimental value.³⁰ It is important also that the value of \( U_{\text{eff}} = 1.875 \text{ eV} \) is sufficient to stabilize the AFM structure with respect to the FM one in contrast to standard DFT calculations.³⁰,³⁴

Due to the Liechtenstein form of the DFT + \( U \) functional,¹⁶ applied to PuO₂, we have to vary the \( U- \) and \( J- \) parameters independently. It was done by varying \( U \)- with the \( J- \) parameter fixed at 1.5 eV and by varying \( J \) at \( U = 3.0 \text{ eV} \), correspondingly. As seen in Fig. 1b, the (001) magnetic structure of PuO₂ is energetically more stable than the (111) one, except for very small values of Hubbard parameter \( U \). It suggests no preference of the (111) magnetic structure, in contrast to UO₂ (see discussion below), for realistic values of \( U- \) and \( J- \) parameters. The difference increases with both parameters, indicating further stabilization of the (001) magnetic structure in a comparison to the (111) one. The energy difference between the two magnetic structures (Fig. 1b) is almost linear for PuO₂, independently of which parameter is varied or fixed. For chosen values of the parameters \( (U = 3.0 \text{ eV} \) and \( J = 1.5 \text{ eV}) \), lattice constants for PuO₂ in the (001) structure are \( a = 5.402 \text{ Å} \) and \( c = 5.513 \text{ Å} \), and lattice parameters in the (111) magnetic structure are \( a = 5.430 \text{ Å} \) and \( \gamma = 88.9^\circ \). In the case of PuO₂ a cubic unit cell becomes elongated in the direction of alternation of magnetic moments. The calculated spin magnetic moments of Pu atoms are 3.81 \( \mu_B \). Experimentally, PuO₂ is cubic with lattice constant \( a = 5.398 \text{ Å} \) and diamagnetic.⁵

In Fig. 2 we present the total densities of states (DOS) for the discussed tetragonal AFM unit cell of PuO₂, when the strong correlation effects are neglected (dashed line) and for the employed values of \( U = 3.0 \text{ eV} \) and \( J = 1.5 \text{ eV} \) (solid line). The DOS clearly demonstrates that PuO₂, like UO₂, tends to be metallic if the strong correlation effects are not treated.

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**Fig. 1** The energy difference between the (111) and (001) magnetic structures for (a) UN as a function of \( U_{\text{eff}} \) (Dudarev’s functional); the inset contains enlarged fragment of the same plot at \( U_{\text{eff}} \leq 2.0 \text{ eV} \); (b) PuO₂ as functions of one of the \( U \) and \( J \) parameters (Liechtenstein’s functional), while another parameter is fixed.
properly, whereas the band gap of 1.5 eV appears for the chosen parameters of the GGA + U scheme. The latter value of the band gap is slightly smaller than the experimental value (1.8 eV).

The case of UO₂ differs from the discussed above trends for UN and PuO₂, reflecting the fact that the ⟨111⟩ magnetic structure in UO₂ is more stable than the ⟨001⟩ one by 62 meV per formula unit at $U = 4.6$ eV and $J = 0.5$ eV. This result confirms the previously published hybrid functional calculations with atomic basis set. Due to the SOI the total energy is reduced almost by 2.66 eV per UO₂ primitive unit cell. This does not affect relative energies of all studied magnetic structures (3-k, 2-k and both ⟨001⟩ and ⟨111⟩ 1-k structures). Relative energies for all considered magnetic structures are provided in Table 1 with respect to the 3-k magnetic structure. The transverse 3-k magnetic structure appears to be the most energetically preferable. This is in accord with inelastic neutron scattering experiments. The 2-k structure proposed by Faber and Lander has just a little bit lower energy (5 meV per formula unit) than the ⟨111⟩ collinear structure but noticeably higher than the transverse 3-k structure.

Both the ⟨001⟩ and ⟨111⟩ collinear structures have unit cells compressed along the direction of alternation of magnetic moment (see Table 1). Magnetic moments of U atoms in both structures point in the same ⟨001⟩ and ⟨111⟩ directions.

All lattice constants in the 2-k structure are different. The lattice of the 2-k structure becomes orthorhombic. As expected (see Section 3 and ref. 18), odd and even oxygen {010} planes are shifted along the Ox axis in the opposite directions. The obtained shift is $\Delta = 9.7 \times 10^{-3} a$ (compare with $\Delta = 2.6 \times 10^{-3} a$ obtained in ref. 10). However, directions of magnetic moments are very different from those suggested in ref. 11: the magnetic moments point almost along the ⟨010⟩ directions, but are slightly tilted towards shorter square diagonal (the squares are perpendicular to the ⟨001⟩ direction). This can be expressed by amplitudes of magnetic waves $M_0 = (0, 1, 0)$. The magnetic moment of 2.06 $\mu_B$ of U ions in the ground state expected from the intermediate coupling of moments. We have to notice that the intermediate coupling theory includes a multi-determinant form of wavefunction, while the present simulations are done in a single-determinant form of wavefunction.

In Fig. 3 we compare the total DOS for different magnetic UO₂ structures. In all considered structures, the highest valence band consists predominantly of U 5f orbitals and the next highest valence band is mostly built from O 2p orbitals. The conduction bands contain U 6d and U 5f orbitals. Our calculations reproduce the band gaps in various magnetic structures of UO₂ (see Table 1) very close to the experimental value (2.0 eV). The band gaps in both considered non-collinear structures are a little larger, by several tenths of eV. In calculations with hybrid

![Fig. 2](image-url)
The total DOS of UO₂ calculated for ⟨001⟩, ⟨111⟩, 2k and 3k structures. The Fermi energy is taken as zero; \( \varepsilon \) is one-electron energy.

functional the band gap for the ⟨111⟩ structure is significantly (by ∼1.5 eV) overestimated.

The U 5f band width is 1.5 eV for the collinear magnetic structures and gets much narrower for the non-collinear cases (0.76 eV and 0.86 eV in case of 2k and 3k structures, respectively). This band splits into two separate sub-bands: U 5f(5/2) and U 5f(7/2) in the 3k structure with a gap of ∼0.1 eV and distance between peaks ∼0.38 eV. The width (∼4.2 eV for ⟨111⟩ structure and ∼4.4 eV for other structures) of O 2p band varies little among considered structures. The gap between O 2p and U 5f valence bands is small, ∼0.3–0.5 eV. As a result, O 2p band shifts, following the narrowing of U 5f valence band, and becomes by ∼0.5 eV closer to the Fermi level in the non-collinear structures than in the collinear ones.

5. Conclusions
We have compared several possible magnetic structures of several key actinides UO₂, UN and PuO₂ based on the GGA + U technique. Our modelling shows that the transverse non-collinear 3-k structure of UO₂ is the most stable one for this material. UO₂ retains a cubic shape in this structure. Two O atoms nearest to each U atom in the direction of its magnetic moment move toward this U atom. This is consistent with both experiment¹¹ and previous computer simulation¹² employing the LDA + U technique within the Wien2k code. It is important that such agreement is achieved with the standard values of Hubbard and exchange parameters (\( U = 4.6 \) eV, \( J = 0.5 \) eV) within Dudarev’s form of the DFT + U approach.¹⁷ Still, a reason for overestimated U atom magnetic moment remains unclear.

The collinear magnetic order causes breaking of cubic symmetry in UN and PuO₂. In contrast to UO₂, neither UN nor PuO₂ show the energetical preference for the rhombohedral distortion. Both materials have the AFM tetragonal ⟨001⟩ structure for a reasonable choice of parameters \( U \) and \( J \). The total DOS of PuO₂ is successfully reproduced using the Liechtenstein form¹⁶ for the Hubbard correction with the parameters \( U = 3.0 \) eV and \( J = 1.5 \) eV. However, as well as in the previous computational studies,⁶–⁹ we obtained that the AFM state of PuO₂ is more stable than the experimentally observed diamagnetic state.⁵

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