



# Modeling of oxygen incorporation in Th, ThC, and ThN by density functional theory calculations



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## ABSTRACT

Oxygen incorporation in nuclear fuel materials is an important issue deserving investigation due to its influence on thermophysical and structural properties. Even if there has been a renewed interest in thorium and thorium compounds in the last years, there is still not much research done on this topic. In this work, we study, by means of density functional theory calculations, the incorporation of oxygen in Th, ThC, and ThN. We analyze the electronic structure finding a characteristic peak to be attributed to oxygen incorporation. We also calculate incorporation and solution energies and obtain migration energies of oxygen through different paths finding that migration through vacancy sites is more energetically favorable than through interstitial ones.

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## 1. Introduction

A renewed interest on thorium and its compounds (like ThC and ThN) has arisen in recent years boosted by research in Generation IV [1] nuclear reactors [2–7]. These materials are candidates to be used as nuclear fuels in these reactors due to their physical advantages: higher melting points, lower thermal expansion coefficients and larger thermal conductivity.

An important issue to be studied in these materials is their relationship with oxygen since these impurities can alter the thermophysical and structural properties, resulting in a decrease in the performance of the nuclear fuel as well as in complications in its manufacturing process and in its later behavior. In the case of UC and UN there are several studies on the role played by oxygen incorporation [8–10]. But, to our best knowledge, there are very few studies on this subject done on Th, ThC and ThN. In the case of Th, Smith et al. studied experimentally the effect of oxygen on the mechanical properties of Th [11]. There are also experimental studies of oxygen reactions in thorium surfaces (see Ref. [12] and

references therein). But there is no theoretical approach available on oxygen incorporation in thorium. In the case of thorium nitride there are neither experimental nor theoretical studies on this matter. In the case of ThC, there is only our own theoretical work, appeared in Ref. [13].

Therefore, in this article we study the effect of oxygen incorporation in Th, ThC, and ThN. We analyze the evolution of the electronic structure and calculate incorporation and solution energies of oxygen in interstitial positions and in vacancy sites. We also analyze the effect of oxygen incorporation in the crystal structure as well as the charge transfer that takes place due to this incorporation. Finally, we calculate oxygen migration energies through different paths.

## 2. Calculation details

The crystal structure of thorium is f.c.c with an experimental [14] equilibrium lattice parameter of 5.085 Å. In our previous work [3] we obtained for  $a_0$  a value of 5.045 Å. ThC and ThN have both a NaCl-type (B1) structure, with only two atoms in the primitive cell, and experimental equilibrium lattice parameters of 5.335–5.344 Å [15] and 5.167 Å [16], respectively. For these compounds we previously obtained 5.335 Å (ThC) [17] and 5.161 Å (ThN) [7].

The incorporation energies were calculated using the following expressions, after Ref. [18],

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a) Incorporation energy of an oxygen atom in a vacancy site

$$E_O^{vac} = E^{N-1} - E_O^N - E_O, \quad (1)$$

where  $E^{N-1}$  is the energy of the supercell with a vacancy,  $E_O^N$  is the energy with the O atom incorporated in the vacancy site and  $E_O$  is the energy of an O atom in an isolated  $O_2$  molecule.

b) Incorporation energy of an oxygen atom in a tetrahedral interstitial position

$$E_O^{int} = E^{N+1} - E^N - E_O, \quad (2)$$

where  $E^N$  is the energy of the calculation supercell without defects and  $E^{N+1}$  is the energy of the supercell with an O atom incorporated in a tetrahedral interstitial position.

Actually, it is physically more important the value of the solution energy, that gives the energy required to create the defect and to incorporate an atom into that defect. It is defined as

$$E^{sol} = E^I + E^F, \quad (3)$$

where  $E^I$  is the incorporation energy (in a vacancy or in an interstitial position) and  $E^F$  is the defect formation energy. In the case of incorporation in an interstitial position the solution and the incorporation energies are the same.

To complete the study of the behavior of oxygen atoms in these materials we calculate the migration energy of oxygen through different paths using the nudged elastic band (NEB) method [34]. The minimum energy path from an initial to a final state is obtained by optimizing a set of intermediate images of the system. The migration energies are obtained through the saddle points of these paths.

Calculations of these energies were carried out with the software package Quantum ESPRESSO [19] based on density functional theory (DFT). For the exchange and correlation potential the Generalized Gradient Approximation in the Perdew–Burke–Erzenhof (GGA–PBE) formulation [20] was used. The reliability of this approximation, for Th and its compounds, has already been proven in several works, for example in ThC [13,17,21,22], in Th [3,23] and ThN [7,24,25]. A norm-conserving Troullier–Martins [26] pseudopotential was used for thorium. This was generated with the *atomic* software available in the same package following Ref. [23]. The pseudopotentials used for carbon [27], nitrogen [28] and oxygen [29] are from the Quantum ESPRESSO pseudopotential library. A 250 Ry energy cutoff was used after checking energy convergence. The simulations were carried out for 64 atoms supercells in the cases of ThC and ThN and for a 32 atoms supercell in the case of Th. These supercell sizes are large enough to avoid spurious interactions due to the periodicity features of the simulation cell. The Monkhorst–Pack [30] (MP) scheme and a  $4 \times 4 \times 4$  k-point mesh were used to sample the Brillouin zone. The integrations in this zone were performed with the Methfessel–Paxton [31] scheme and with an energy smearing of 0.02 Ry. The atomic positions were fully relaxed till forces were less than 0.026 eV/Å. The migration paths were calculated with the NEB method as implemented in the software package [19]. We have assumed a non magnetic ground state for ThN [24,32], ThC [15,25], and Th [33].

### 3. Results and discussions

In the following, we present the effects that oxygen incorporation has on the electronic structure of the systems under study and the results obtained for the incorporation and solution energies of

oxygen in these materials. Then, we discuss the resulting atomic displacements and charge transfers. Finally, we study oxygen migration.

#### 3.1. Electronic structure

In Fig. 1 we show the total densities of states (DOS) as a function of energy for ThN (panel (a)), ThC (panel (b)), and Th (panel (c)). For each of these materials we compare the DOS with and without an oxygen impurity in a tetrahedral interstitial position.

For the three systems the main difference between the DOS in the two situations is a peak appearing around  $-6$  eV for ThN (Fig. 1 (a)) and Th (Fig. 1 (c)) and around  $-5$  eV for ThC (Fig. 1 (b)). These peaks are relatively small due to the small fraction of incorporated oxygen atoms.

In Fig. 2 (a) we show DOS curves for ThN without and with an oxygen atom incorporated in a N vacancy. This last curve has a peak near  $-6$  eV which is absent in the one of the perfect lattice. In Fig. 2 (b) DOS curves for ThC are presented. In this case the presence of oxygen in the vacancy site reflects in the peak at  $-5$  eV.

There is almost no difference among the DOS without defects and with an oxygen incorporated in a Th vacancy, for the three materials.

In Fig. 3 we show the projected local densities of states on the oxygen 2p orbitals for the cases with incorporated oxygen of Figs. 1 and 2. We observe that the peaks around  $-6$  eV for Th and ThN and around  $-5$  eV for ThC are to be attributed to this orbital.

In Fig. 4 we present projected densities of states (PDOS) on thorium atoms that are first nearest neighbors to an oxygen atom in a N vacancy (Fig. 4 (a)) in the case of ThN and in a C vacancy (Fig. 4 (b)) in the case of ThC. These are to be compared with the PDOS of thorium atoms in lattices without oxygen impurities. We plot only for Th-d orbitals because it is the only case for which there is an important modification in the DOS due to the presence of the oxygen atom. We observe peaks at  $-6$  eV for ThN and  $-5$  eV for ThC and this points towards hybridization of these orbitals with the p orbital of oxygen.

In Fig. 5 the PDOS of thorium, carbon, and nitrogen atoms that are first nearest neighbors of interstitial oxygen atoms in Th, ThC, and ThN are shown. We observe that peaks around  $-6.5$  eV appear for Th-d and N-p orbitals due to hybridization in the case of ThN (See Fig. 5). In Fig. 5 (b) hybridization peaks around  $-5.5$  eV for Th-d and C-p orbitals in ThC are observed. Finally, in Fig. 5 (c) we observe that the most notorious feature in the case of pure Th is a

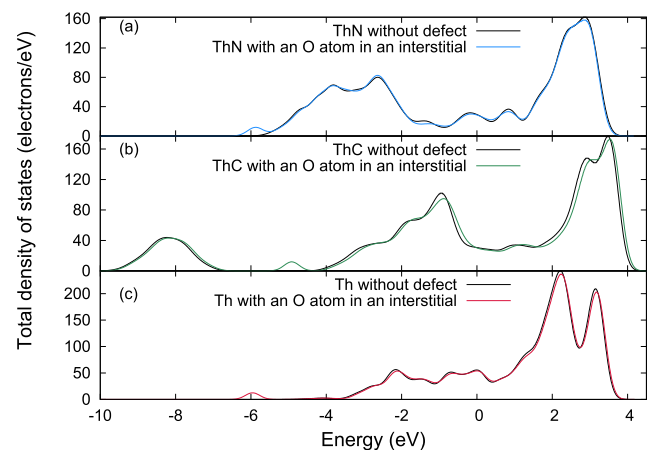
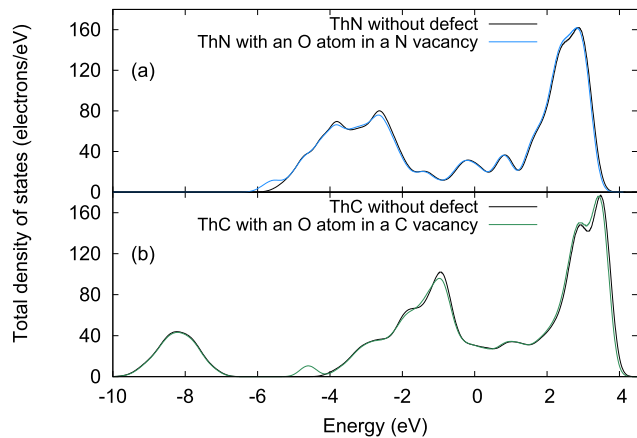
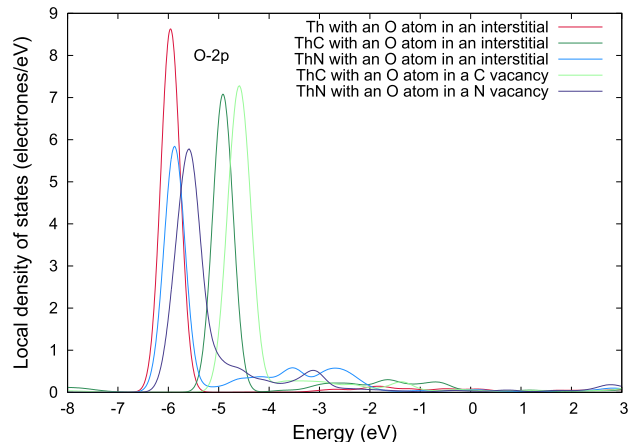


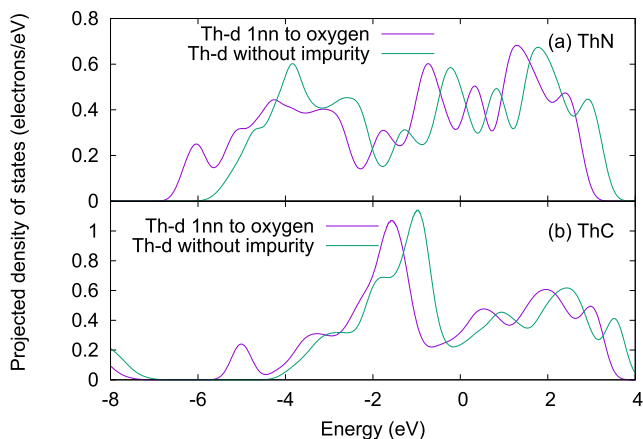
Fig. 1. Total densities of states for a lattice without defects and a lattice with an oxygen atom incorporated in an interstitial tetrahedral position. (a) Thorium nitride. (b) Thorium carbide. (c) Thorium.



**Fig. 2.** Total densities of states for a lattice without defects and for a lattice with an oxygen atom incorporated in a vacancy site. (a) Thorium nitride lattice with an O atom on a N vacancy. (b) Thorium carbide lattice with an O atom on a C vacancy.



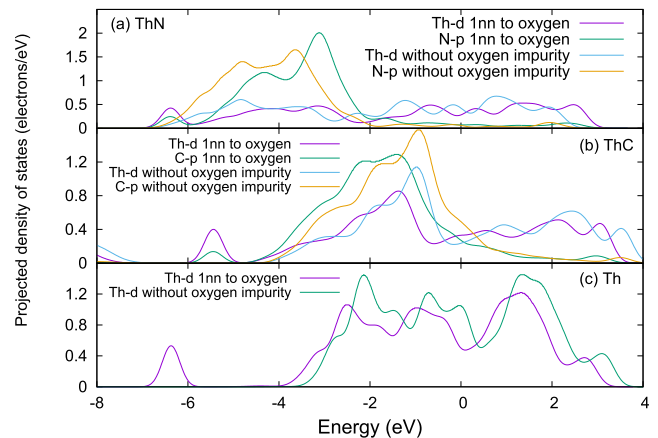
**Fig. 3.** Projected local densities of states on an oxygen atom in interstitial sites and in a vacancy site.



**Fig. 4.** Projected local densities of states on thorium atoms first nearest neighbors to an oxygen atom in a C or N vacancy or on thorium atoms in a lattice without oxygen impurities for ThC and ThN. (a) Th-d orbitals in ThN. (b) Th-d orbitals in ThC.

peak around  $-6.5$  eV, also due to hybridization with oxygen p orbitals.

Peaks in the DOS around  $-6$  eV are also present in UN and UC. Kotomin et al. studied UN with oxygen impurities and found a peak



**Fig. 5.** Projected local densities of states on the first nearest neighbors (1nn) to an interstitial oxygen and for a lattice without oxygen impurities as a function of energy for Th, ThC, and ThN. (a) Th-d and N-p orbitals in ThN. (b) Th-d and C-p orbitals in ThC. (c) Th-d orbital in Th.

around  $-6$  eV for oxygen atoms in N vacancies [35]. Lopes et al. also observed this peak in the DOS of UN with an oxygen impurity [36]. Bocharov et al. also obtained this peak in a study of surface vacancies and oxygen impurities in UN [37]. Experimentally this peak was observed by Black et al. in thin UN films [38] and by Eckle et al. in thin UN and UC films [39]. All these works coincide in pointing out that oxygen p orbitals are responsible for this feature. With the help of ultraviolet photoelectron spectroscopy the presence of this peak could provide a way to detect oxygen impurities in these materials.

### 3.2. Incorporation and solution energies

In Table 1, we present incorporation energies of oxygen in tetrahedral interstitial defects and in Th, C, and N vacancies of systems under study using equations (1) and (2). Lower energy values imply a more favorable incorporation position and a negative energy indicates that the incorporated atom is energetically stable in the lattice. The results for ThC were calculated in a previous work [13] and are presented here for comparison. We observe that in Th the most energetically favorable position is a tetrahedral interstitial. For ThC, it is a C vacancy and for ThN, it is a N vacancy. The incorporation energies of an oxygen atom in Th vacancies of ThC and ThN are positive suggesting energetically unstable positions. Freyss [18] found in UC a similar behavior as in ThC. An oxygen atom in a C vacancy or in an interstitial position has negative incorporation energy while in an uranium vacancy it is slightly positive. He also found that an oxygen in a C vacancy has the lowest incorporation energy. Kotomin et al. [35] and Lopes et al. [36] both found in UN a similar behavior as in ThN, where an oxygen atom in a N vacancy has lower incorporation energy than in an interstitial position and both energies are negative.

In Table 2 we present solution energies calculated using equation (3) for the different situations. Vacancy formation energies were previously calculated, for Th in Ref. [3], C and Th vacancies in ThC in Ref. [22] and, N and Th vacancies in ThN in Ref. [7]. We observe that taking into account the cost of vacancy formation in Th, the energy necessary to incorporate oxygen in the vacancy is positive. In ThC, a C vacancy is still the most energetically favorable site for oxygen incorporation. In ThN, the most energetically favorable site is an interstitial position. If we take into account the cost of  $O_2$  bond breaking, that is 5.12 eV, only the interstitial position in Th and a C vacancy site in ThC remain having negative energy.

**Table 1**

Incorporation energy (eV) of an O atom in tetrahedral interstitial and vacancy defects in Th, ThC and ThN.

	Interstitial (eV)	Vacancy (eV)	
Th	−5.25	−2.09	
ThC	−3.49	0.25 (Th)	−6.45 (C)
ThN	−3.73	1.29 (Th)	−6.58 (N)

**Table 2**

Solution energy (eV) of an O atom incorporated in tetrahedral interstitial and vacancy defects in Th, ThC and ThN.

	Interstitial (eV)	Vacancy (eV)	
Th	−5.25	0.01	
ThC	−3.49	6.09 (Th)	−6.30 (C)
ThN	−3.73	5.26 (Th)	−2.89 (N)

### 3.3. Defect-induced lattice distortions

Here, we analyze the effect of oxygen incorporation in the structure of Th, ThC, and ThN lattices. The oxygen atom incorporated in a tetrahedral interstitial position produces an outward displacement of 0.09 Å of the four nearest thorium atoms in Th. In ThC and ThN, the oxygen atom produces an outward displacement of 0.28 Å of the four nearest carbon atoms and of 0.27 Å of the four nearest nitrogen atoms, respectively. No displacement of the four nearest thorium atoms occurs. When the oxygen atom is incorporated in a thorium vacancy in the Th lattice, it yields an inward displacement of 0.14 Å of the twelve nearest thorium atoms. There is a 0.37 Å outward movement of the four nearest neighbor carbon atoms due to oxygen incorporated in a thorium vacancy in ThC. For ThN this movement is of 0.29 Å. The oxygen atom incorporated in a carbon or a nitrogen vacancy drives insignificant movements of the nearest atoms of the vacancies.

### 3.4. Charge transfer

In Table 3 we present the charge transferred to incorporated oxygen atoms in interstitial positions and in vacancy defects obtained through a Bader [40] analysis for the systems under study. In the case of pure ThC the charge transfer from Th to C is  $-1.81e$  and in the case of ThN the charge transfer from Th to N is  $-1.72e$ . We observe that the charge transfers are similar for ThN and ThC, the largest transfer takes place in the case of C and N vacancies, which coincides with the most energetically favorable incorporation sites. In UC [18] and UN [35] a similar behavior was observed. For Th, the charge transfer in the interstitial case is larger than in the vacancy case, similar as in ThC and ThN.

### 3.5. Migration of oxygen impurities

Finally, we study the diffusion of oxygen through vacancy and interstitial paths for Th, ThC, and ThN. From the saddle point of these paths we obtain the migration energy. In the case of vacancy paths, we only calculate migration through carbon and nitrogen vacancies, as incorporation of oxygen in Th vacancies is

**Table 3**

Charge transferred to an incorporated oxygen atom in interstitial positions and in vacancy defects obtained through Bader analysis for Th, ThC and ThN.

	Interstitial	Vacancy	
Th	−1.41e	−1.17e	
ThC	−1.30e	−0.87e (Th)	−1.41e (C)
ThN	−1.32e	−0.96e (Th)	−1.45e (N)

energetically very unfavorable.

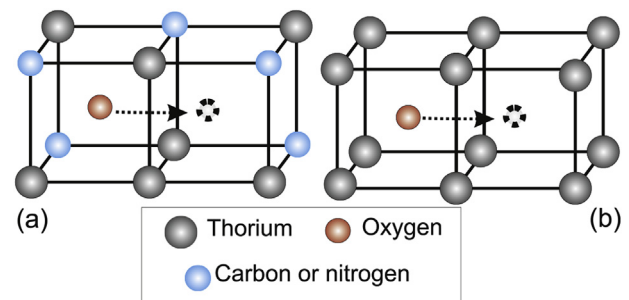
In Fig. 7 we present the results of the NEB calculations for migration of an oxygen atom from one tetrahedral interstitial position to another for Th, ThC and ThN (see Fig. 6). We observe that the oxygen migration energy through Th is much smaller than through ThC and ThN, which have higher energetic barriers. In Table 4 the migration energies for these migration paths are presented.

In Fig. 8 we show the energetic barriers for a oxygen atom migrating from one vacancy to another. In the case of ThC the vacancy is a carbon one and for ThN it is a nitrogen one. We observe that the highest energetic barrier is for ThN. In Table 4 the migration energies for these migration paths are shown.

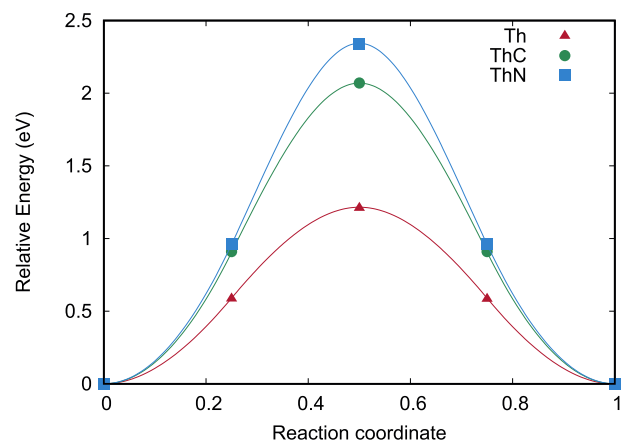
We observe that oxygen migration through vacancy paths is energetically more favorable than through interstitials in the cases of ThC and ThN. For oxygen diffusion in UN, Lopes et al. found that migration through N vacancies is more favorable than through interstitial positions [36], similar to what happens in the systems under study.

## 4. Conclusions

In summary, we studied, by means of first principle calculations, oxygen incorporation in Th, ThC, and ThN. We found a peak near  $-6$  eV that characterizes oxygen incorporation. This feature appears for oxygen incorporated in a N vacancy and in an interstitial position in ThN, and also in a C vacancy and in



**Fig. 6.** Oxygen migration path from one tetrahedral interstitial position to another. (a) ThN or ThC NaCl type structure. (b) Thorium FCC.



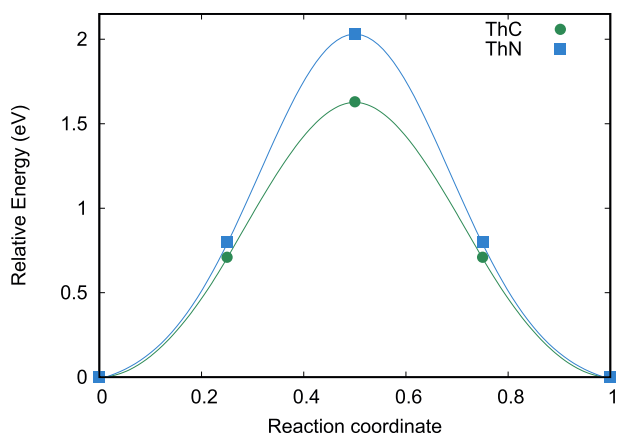
**Fig. 7.** Relative energy (eV) as a function of the reaction coordinate for the migration of an oxygen atom from a tetrahedral interstitial position to another one in Th (red triangles), ThC (green circles), and ThN (blue squares) lattices. The energies are relative to the initial configurations. The lines are an interpolation of the path energy profile that goes exactly through each image. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)



**Table 4**

Migration energy (eV) for an oxygen atom through interstitial and vacancy paths for Th, ThC, and ThN.

Materials	Defects	$E_m$ (eV)
Th	Int	1.21
ThC	Int	2.07
	Vac (C)	1.63
ThN	Int	2.34
	Vac (N)	2.03



**Fig. 8.** Relative energy (eV) as a function of the reaction coordinate for the migration of an oxygen atom through a vacancy path. For ThC (green circles) the migration is from a C vacancy to another one. For ThN (blue squares) the migration is from a N vacancy to another one. The energies are relative to the initial configurations. The lines are an interpolation of the path energy profile that goes exactly through each image. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

interstitial positions in ThC and in Th.

We also calculated incorporation and solution energies and found that the most favorable sites for oxygen incorporation are interstitial positions for Th, C vacancies in the case of ThC and N vacancies for ThN. We compared these results with UC and UN. If the energy cost of defect formation is taken into account the interstitial positions in Th and C vacancies in ThC remain the most energetically favorable sites for incorporation in each material, but in the case of ThN the interstitial position is now the most energetically favorable site.

We also analyzed the effect of oxygen incorporation in the structure of Th, ThC, and ThN lattices. We found that the largest atomic displacements correspond to the four carbon nearest neighbors atoms of an oxygen incorporated in a Th vacancy.

We studied the diffusion of oxygen through a vacancy and an interstitial paths for Th, ThC, and ThN. In the case of migration through interstitial positions the oxygen migration energy through Th is much lower than through ThC and ThN. We also observed that oxygen migration through vacancy paths is energetically more favorable than through interstitials for ThC and ThN.

Summarizing, in the case of oxygen incorporation in thorium and its compounds with C and N, and within the limitations of this

study, we draw the conclusion that ThN is the more suitable as a nuclear fuel due to its larger solution energy and its larger diffusion energy barrier. This means ThN presents a smaller probability of oxygen incorporation and diffusion being because of this better than ThC and Th in avoiding oxygen contamination.

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