**Comments from the editors and reviewers:**  
-**Reviewer 1**  
  
  - The authors study the TDE of the different elements in UO2, by means of molecular dynamics. The paper is mostly written in a good manner, without any major language problems. The method used in this paper is appropriate for this kind of investigation, with some small possible questions about the analysis. However, in its current form, this manuscript is a very incremental work with very low statistics, and therefore would be more suitable as a conference paper. In addition, the work cannot be compared to experiments in its current form, so more simulations are needed to be able to validate which potential is giving the correct answer. Below are some comments and questions about the manuscript, both some major issues and some minor issues.

Major issues:

As said, the main limitation of the paper is the very few investigated directions of the PKA, which render the results uncomparable with experiments, where the average should be calculated. Only 40 simulations are not enough, especially at high temperatures, where the thermal fluctuations are major. Also the error bars are missing, and I assume they could be quite large, considering the low statistics. These simulations are not that computationally heavy, so more should be done, to be able to draw the conclusions that are written in the manuscript.

Some considerable changes have been made to the manuscript. Datasets have been expanded to 100 simulations for each PKA direction, PKA atom type, energy and potential. It has been included that 100 simulations is a reasonable amount to achieve a converged result. Additionally, the directions have been modified to investigate three high symmetry directions, three low symmetry directions, and a set of random directions. Finally, regarding error bars, we considered that it was not beneficial to provide them. For probability distributions, we are using a data set that is binomial, yielding either a 1 (yes defect) or a 0 (no defect). Thus, the standard deviation increases are the average value tends towards 0.5 and decreases towards both 0 and 1. This does not provide any descriptive information on the dataset, but only provides a characteristic of binomial distributions. We also believe that the addition of a chart to indicate convergence of the data provides sufficient indication of statistical significance.

You modified the potential, and "assume" that the properties are the same. I would insist on checking this claim, as you are doing simulations at high temperatures and that it is not good manner to "expect" that something is something. Better to do benchmark tests.

This has been verified and the text discussing the modifications to the potentials has been updated. A full inclusion of fundamental properties, comparing ZBL-splined potentials to original potentials, seemed excessive to include in this manuscript. If the referee wishes to include such a thorough study, this can be expanded and perhaps attached as an appendix. However, it is currently not present within the manuscript.

I am not really convinced about the effect of the quenching of the cells, I think that that could affect the end results, as the interatomic potential probably have some very drastic changes in elastic moduli and so on. So the stable configurations at elevated temperatures are maybe not the same at 0K.

The intention behind quenching the cells is to reduce noise from thermal motion. Systems at 1500K in UO2 have sufficient thermal motion to yield spurious results when defect analyses are performed. By performing a somewhat rapid quench, the defect structures are frozen in, and analyses are able to be performed with zero thermal motion. The defect configurations may change (an octahedral moving to a dumbbell perhaps), but the population of defects will remain the same. The paper has been expanded to explain this.

The use of voronoi analysis for the defects sounds a bit strange, as the authors generate the cells at zero kelvin, then heat up the cell, and after the recoil event cool it down, and then analyze the results. I would assume that the thermal motion of atoms and maybe some collective motion of atoms would render the end results completely wrong. Would it not be better to use for instance a adaptive wigner-seitz analysis, that would detect the collective motion etc.

The use of a Voronoi cell to determine defects has become somewhat standard practice and is somewhat widespread in the literature. The authors feel that a Voronoi cell analysis and a Wigner-Seitz analysis are essentially the same technique, but only under different names. If we misunderstand or need to revise our nomenclature, we will gladly do so. In the crystalline samples collective motion would either be a diffusion process (unlikely without the presence of defects on the timescales studied) or a drift of the entire sample (which is not observed in our simulations).

Minor issues:

Was electronic stopping applied or not in the simulations, there is no mention about that.

Electronic stopping not applied. At such low energies this should not be an issue. A sentence has been included indicating this.

On page 5 there is some strange equation without explanation, "sum of KE - 1 eV"

This equation has been further explained in the text.

Most references are wrong, both lower-case letters are incorrectly used and some text is incorrectly italic / non-italic

References have been verified and formatted.

In the text, most of the subscripts are italic, even though that is incorrect

The subscripts and terms including subscripts have been modified accordingly.

The heading is wrong, UO2 should not be italic (also found in the text)

The italicization of UO2 has been corrected.

-**Reviewer 2**  
  
  -

The authors investigate via molecular dynamics simulations the threshold displacement energy (TDE) of both uranium and oxygen atoms in UO2 matrix. As stated by the authors, beside the importance of this topic for studying the irradiation properties in nuclear fuels very few studies are dedicated to this calculation and only one experimental measurement has been carried out in the seventies. Therefore, the subject is really of importance and is well targeted for the journal of nuclear materials. The authors provide three different definitions for the TDE and calculate them systematically according each definition and three different interatomic potentials. Overall, the paper is understandable and well organized even if the legends of the figures are small which render them hard to read.

However, there are still some issues and points that need clarification before this paper can be suitable for publication in the journal of nuclear materials. I will list them as they appear in the text.

·         In the introduction for the NRT study with two components, the authors could refer to the work of Crocombette (JNM 474 (2016) 134) who investigates this point.

We have included a sentence referred to the paper by Crocombette and the relevance of NRT to a non-monoelemental system.

·         Introduction, 5th paragraph. It should read “… to remove our atoms from its lattice site…”

It is unclear which sentence the reviewer is referring to. However, if further edits need to be performed, we will gladly make the needed corrections.

·         In the interatomic potential. The authors study systematically three interatomic potentials: Basak, Yamada, and Yakub. I do understand that studying more interatomic potentials is time consuming, yet these three potentials are not really different to one another and provide very similar results for most of thermodynamics and structural properties. At least a discussion about the choice of not using other potentials like Cooper or Morelon that yield to different values on some properties such as mechanical or transport properties will be useful.

We have expanded the work greatly to include both the Morelon and Cooper potentials, while excluding the Yamada potential, due to its similarities with the Yakub.

·         In computational details. The time for relaxation at high temperature is set to 5.5 ps with extra relaxation time for quenching to 0 K of 14 ps. How this relaxation time compares to the time of Frenkel pair recombination? This is important for the first definition of the TDE. At least a discussion on this issue is necessary.

Further discussion on relaxation time and quench time has been provided.

·         General remark. It is mentioned that 40 independent simulations are carried out to ensure statistical significance of the data set. However, it is unfortunate that none of the figures provide error bars (for instance standard deviation). This is very important to discuss the results and need to be added.

The work has been modified to include 100 simulations for each data point. A discussion of the error is included in the text. Regarding inclusion of error bars, we concluded that it was not beneficial to provide them. For probability distributions, we are using a data set that is binomial, yielding either a 1 (yes defect) or a 0 (no defect). Thus, the standard deviation increases are the average value tends towards 0.5 and decreases towards both 0 and 1. This does not provide any descriptive information on the dataset, but only provides a characteristic of binomial distributions. We also believe that the addition of a chart to indicate convergence of the data provides sufficient indication of statistical significance.

·         Figure 1. The abscissa should be in real time not time step, especially because time step changes during this simulation.

This figure has been remade to show excess kinetic energy as a function of time, not timestep.

·         Results 3rd paragraph. It should read “PKAs (Ed[O]) is 20 eV…”

The text has been modified.

·         Section 4.2 discusses about probability of lattice site displacement. I do not understand clearly what is the difference between this definition and the activation energy of self-diffusion (migration energy + defect formation energy). Could at least the authors discuss this point.

A sentence pointing out the difference between self-diffusion and TDE has been added to the introduction section.

·         Section 4.3. The definition of “permanent” needs to be specified. The time frame of the MD simulation is limited to few picoseconds which is short compared to the time of recovery of some Frenkel pairs that can be up to hundreds of picoseconds (Devynck PRB 85 (2012) 184103). Therefore, the TDE could change.

The reviewer makes an excellent point. The text has been modified to include a discussion on the nature of the terms permanent and stable and emphasis has been drawn to the limited time scale of the simulations.

·         The conclusion is rather unclear. What is according to the authors the most significant definition for TDE? At least provide a discussion. Here error bar on the results could help drawing trends.

Discussion of different definitions of Ed has been included in a more developed discussion section.

-**Remarks by the associate editor**  
  
  - The authors write "Soullard [7,8] determined that the threshold displacement energies in UO2 are 20 eV for oxygen primary knock-on atoms (PKAs) and 40 eV for uranium PKAs].

I invite them to read carefully the reference by Soullard (JNM 1985). the actual displacement energy of oxygen HAS NOT BEEN MEASURED by Soullard.  At page 193 of Soullard's paper one can read :

"As the experiments do not allow the displacement threshold energy of oxygen atoms in UO2 to be determined, their production rate was then calculated by assuming that: Ed2 = Ed1/2. This assumption is based on the fact that 8 U-O bonds must be broken to create a uranium defect in UO2, which has the fluorine structure when only 4 of these bonds are broken to create an oxygen defect."

We thank the editor for the clarification, and we have revised the text to accurately reflect the state of the experimental data.

I am unaware of any measurements of the displacement energy of oxygen in UO2. So basically the displacement energy of oxygen in uranium oxide is unknown! For years everyone has done as if it was well known to be 20eV (which is a reasonable, if not measured, value) but there is no proof. The authors must at the very least acknowledge this point.

The text has been modified to more clearly illustrate this point.

-Concerning the remark of the second referee on the lifetimes of Frenkel Pairs in UO2, the authors could look at "L. Van Brutzel, A. Chartier, and J. P. Crocombette, Phys. Rev. B 78, 024111 (2008)".

We thank the editor for pointing out this reference. It has been included in the discussion on permanence of defects and displacement.