**Comments from the editors and reviewers:**  
-**Reviewer 1**  
  
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The authors present their work on threshold displacement energies (TDE) in uranium metal. This work is interesting and

valuable, as TDEs are a fundamental property of that material that can also be of great importance to parameterise

mesoscale or macroscopic models. I also think that this will be of interest to JNM readers. Overall, I recommend this

article to be published provided that the authors address the points below.

p.4: It would be useful to have the approximate physical lengths of the simulation boxes, particularly considering that

the lattice parameters of alpha-U and gamma-U are not mentioned in that paper.

p.4: The authors mention a range of 35.3º for phi, divided into 4º intervals, surely at least one of these numbers is

inaccurate.

p.6: It is mentioned that the simulations have been done at 800 K and 1000 K. Why have these temperatures been chosen?

p.6: A standard arithmetic average over the different directions is problematic from a statistical point of view. Using

the scheme presented in p.4, the directions are not uniformly distributed. If the authors have used the correct

averaging presented in Nordlung et al. 2006, they should make it explicit, if only to help readers doing it properly in

the future.

p.6: I am not entirely sure why a polynomial was fitted to the average data. I assume that this was done to calculate

the TDE more accurately, but this is unclear. It would be interesting to have the data points along with the polynomial

on figure 3, to show the quality of the fit.

p.6: The authors make the point that the Frenkel pair (FP) formation probability is not a step function at finite

temperature. Then, it would be nice to show the curves for the two considered temperatures in figure 3.

p.9: The authors discuss direction-dependent changes in TDE. It would be interesting to discuss this in terms of the

crystal structure (neighbour and interstitial sites positions). As it is, the numbers do not give much insight on why

specific directions have particularly large or low TDEs.

p.9: The authors emphasise the importance of selecting a good potential, but in the following sentence explain that

because of the lack of experimental data it is impossible to assess the quality of the potentials. It seems that

instead of arguing for selecting the right potential that reproduces experimental numbers, the authors really argue for

using different potentials to try to estimate systematic error caused by one particular potential.

p.10: The authors have done the simulations at two temperatures, they should show the resulting averaged probabilities

on figure 5, this would give more information than simply the TDE reported in table 2.

p.10: Discussions on the ZBL potential do not really belong in the results section. I would suggest adding a section

describing the potentials before the results section. It would also be useful to have the functional forms of the

different potentials, and possibly the exact potential parameters used, in the interest of helping other people

reproduce these results. Alternatively, the LAMMPS definitions of the potentials used would be valuable supplementary

information. It would also be useful for context to provide basic materials properties predicted by the three

potentials such as lattice parameters and cohesive energy of the considered structures when appropriate. To be honest,

the dimer energy predicted by the UMo ADP potential as shown in figure 6 does not inspire much confidence.

p.11: The way the error ranges have been calculated and the authors obtained the 68% confidence energy intervals is

unclear and should be detailed. In any case, the intervals reported in table 2 are not centred on the mean, and

therefore are not confidence intervals in the standard sense.

p.12: It might be useful to clarify that the FP energy calculated that way correspond to unbound FP, which is not

necessarily the case of the FP formed during the TDE simulations.

p.13: The uncertainties should be added to the defect energies in table 3.

p.18: The temperatures considered for alpha-U are 600 K and 800 K. The authors should explain why these values have

been chosen, and why are they different from the temperatures chosen for gamma-U.

p.18: As in the case of gamma-U, standard, unweighted arithmetic averaging is probably inaccurate.

p.19: Figure 11 shows peaks for some of the FP formation probability (notably around 30 eV, with one reaching 0.9

before decreasing below 0.8). This should be discussed and linked with structural features (concerned directions and

mechanisms involved). This figure also shows local minima (e.g around 100 eV and 120 eV) which suggest sampling issues.

p.20: As in gamma-U, the direction dependence of the TDEs should be discussed in terms of crystal features.

p.21: The uncertainties should be added to the defect energies in table 5.

p.22: It would be useful to add the DFT defect formation energies from the literature to the tables 5 and 6 where they

could be directly compared with the MD results.

Finally, there were a couple of minor typos and awkward sentences that could benefit from additional proofreading.

-**Reviewer 2**  
  
  - I recommend the paper for publication after minor corrections in accordance with the following remarks.

1. Page 6, lines 5-6 of item 3.1. It is reasonable to point out that results shown in Fig.2 were obtained for temperature of 800K.
2. Page 13, line 6. The units of energy should be given.
3. Page 15, lines 1-3. It is desirable to give more details what r2 is and how D0 and Em are calculated.
4. Page 15, second line below Eq.(2). Are cintand cvac really energies?
5. Page 18, third line of item 3.2. Only one potential is used for α-U.
6. Page 19, Fig. 11. Sharp peaks are observed in probability curves for many directions. What is the cause? Some curves cross the line of probability of 0.5 several times. How was displacement energy evaluated in such cases? There are a few resembling peaks in Fig.2. But they are not so sharp there.
7. Page 22, lines 2-4 below Table 6. In my opinion, formation energy can be easily calculated for zero temperature to compare with DFT results.