We thank the reviewer for their constructive comments and positive feedback. The following edits have been made to the manuscript:

1. Inclusion and discussion of *[A. Landa, P. Söderlind, P.E.A. Turchi, Density-functional study of the U-Zr system, J. Alloys Compd. 478 (2009)103-110;* [*https://doi.org/10.1016/j.jallcom.2008.12.052*](https://doi.org/10.1016/j.jallcom.2008.12.052)*]* in the literature review.
2. The SCAILD results from Söderlind *[P. Söderlind, A. Landa, A. Perron, B. Sadigh, and T.W, Heo, Ground-state and thermodynamical properties of uranium mononitride from anharmonic first-principles theory, Applied Sciences, 9 (2019) 3914;* [*https://doi.org/10.3390/app9183914*](https://doi.org/10.3390/app9183914)*]* were included in the discussion of results.
3. The DFT + OP + SCAILD results from Söderlind *[P. Söderlind, A. Landa, E.E. Moore, A. Perron, J. Roehling, J.T. McKeown, Appl. Sci. 13 (2023) 2123;* [*https://doi.org/10.3390/app13042123*](https://doi.org/10.3390/app13042123)*]* were briefly discussed.

Reviewer #2: The authors of this manuscript present AIMD results of the thermodynamic properties of the δ-UZr2 phase in the U-Zr metallic fuels for the liquid metal fasts breeder reactors. It is well known, [21] and the references to it, that during the burn-up process, composition of U in the fuel rod decreases resulting in a subsequent increase of Zr composition in the "hot" center and "cold" periphery zones of the fuel rod. The excess Zr in the periphery zone is important because Zr interacts with the stainless-steel cladding by suppression interdiffusion of bred minor actinides, especially Am. The authors correctly mention in the Introduction that a higher Zr content in the periphery "will likely lead to an increased presence of the δ-phase". These factors make the study of the δ-UZr2 phase very relevant.

For the first time the authors found the nature of the magnetic ground state (anti-ferromagnetic) of the δ-UZr2 phase. Following the arguments made by Söderlind et al., [27,48], the authors confirm that applying of an on-site Coulomb interaction term (Hubbard U > 0) is not necessary to correctly describe the ground state of the δ-UZr2 phase within the generalized gradient approximation (GGA) for the electron exchange and correlation energy functional. The authors emphasize that LDA+U study of Xie et al. [23] is wrong because (it) "introduces an unphysical strong spin polarization" that is contradictory to the conclusions of Söderlind et al., [27,48] and experimental results. On the topic of magnetism for uranium, the ground-state orthorhombic (alpha) phase is non-magnetic, but uranium is very close to a magnetic instability. Changing its crystal structure and/or expanding the volume through thermal expansion can lead to formation of magnetic moments. It was shown that in gamma-U (high temperature bcc phase) spin and orbital magnetic moments are formed and their contributions to the thermodynamics are significant. This result is consistent with that of the present paper. A short discussion of this would fit the paper well, and if the authors decide to include that, the appropriate reference is listed below as Ref. I.  
  
The calculated formation energy, equilibrium atomic volume, thermal expansion coefficient, and the elastic constants of the δ-UZr2 phase are in good agreement with the experiment. The topic of the manuscript meets the interest of the broad readership of the Journal of Nuclear Materials, especially those who work in the field of liquid metal cooled fast breeder nuclear reactors. The manuscript is well written, the work seems well executed, and accordingly, I recommend its publication after some changes in the Reference List.  
  
In the previous publications:  
A.P. Moore, B. Beeler, M. Baskes, M. Okuniewski, C.S. Deo, Atomistic Ordering in Body Centered Cubic Uranium-Zirconium Alloy, Mater. Res. Soc. Symp. Proc. Vol. 1514, <https://doi.org/10.1557/opl.2013.517>  
A.P. Moore, B. Beeler, C. Deo, M.I. Baskes, M.A. Okuniewski, Atomistic modeling of high temperature uranium-zirconium alloy structure and thermodynamics, Journal of Nuclear Materials 467 (2015) 802-819; <http://dx.doi.org/10.1016/j.jnucmat.2015.10.016>  
A.P. Moore, C. Deo, M.I. Baskes, M.A. Okuniewski, Atomistic mechanisms of morphological evolution and segregation in U-Zr alloys, Acta Materialia 115 (2016) 178-188; <http://dx.doi.org/10.1016/j.actamat.2016.05.052>  
the authors mentioned that the first published density functional theory (DFT) simulation of the U-Zr system was performed by Landa et al. [II], including the correct description of the partial ordering, equilibrium volume, and negative heat of formation of the δ-UZr2 phase. I think that the authors should reflect the paper [II] in their article.  
The author mentioned the paper [41] where a non-zero temperature simulation was required to obtain the appropriate ground state magnetic ordering and more accurate electronic and thermal properties of uranium mononitride (UN). The authors should mention the paper [III] where FPLMTO-GGA and SCAILD were applied to study the thermodynamic properties of UN at low and high temperatures.  
  
I. P. Söderlind, A. Landa, E.E. Moore, A. Perron, J. Roehling, J.T. McKeown, Appl. Sci. 13 (2023) 2123; <https://doi.org/10.3390/app13042123>  
II. A. Landa, P. Söderlind, P.E.A. Turchi, Density-functional study of the U-Zr system, J. Alloys Compd. 478 (2009)103-110; <https://doi.org/10.1016/j.jallcom.2008.12.052>  
III. P. Söderlind, A. Landa, A. Perron, B. Sadigh, and T.W, Heo, Ground-state and thermodynamical properties of uranium mononitride from anharmonic first-principles theory, Applied Sciences, 9 (2019) 3914; <https://doi.org/10.3390/app9183914>