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Dear Editorial Board,

Journal of Nuclear Materials

On behalf of my co-author and myself, I am hereby re-submitting our manuscript, entitled ``*Magnetism and finite temperature effects in UZr2: A Density Functional Theory Analysis”* to your journal.

This article presents a computational study on the structural, thermophysical, and magnetic properties of δ-UZr2. Our research investigates the complexities associated with modeling the δ phase of the U-Zr alloy. In contrast to the previous density functional theory (DFT) calculations on this phase prevalent in existing literature, we have successfully eliminated the DFT-associated artificial ferromagnetic effects. This was made possible through the application of *ab initio* molecular dynamics at finite temperatures. Our investigation underscores the critical role of magnetism control within the modeling of the U-Zr system in achieving precise results for structural characteristics and thermophysical properties, including atomic volume, thermal expansion, and heat capacity. Our results are consistent with the recent neutron-diffraction experimental results reported in the literature.

We have addressed all reviewer comments, the description of which is included in the response to reviewers document.

Sincerely,

Benjamin Beeler