**Cover letter**

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Dear Editor,

We wish to submit an original research article entitled “Ab initio molecular dynamics of paramagnetic uranium mononitride (UN) using disordered local moments” for consideration in the journal *Computational Materials Science*. We confirm that this work is original and has not been published elsewhere, nor is it currently under consideration for publication elsewhere.

This work presents an investigation of the thermophysical properties of paramagnetic uranium mononitride (UN) using *ab initio* molecular dynamics (AIMD) simulations combined with the disordered local moment (DLM) approach. This methodology accurately captures the high-temperature paramagnetic state of UN, addressing the limitations of standard density functional theory (DFT) models. The AIMD+DLM model consistently predicts a cubic crystal structure for UN across all considered temperatures, aligning with experimental observations of its paramagnetic phase. Key thermophysical properties, including the lattice parameter and specific heat capacity, are computed and compared to experimental data. The calculated lattice parameter is somewhat underestimated relative to the empirical correlation, consistent with prior studies modeling UN as a ferromagnetic (FM) or antiferromagnetic (AFM) material. The specific heat capacity exhibits overestimation at low temperatures (300--500 K) and slight underestimation at higher temperatures, while closely following the experimental trend. These results highlight the accuracy and utility of the AIMD+DLM framework in modeling paramagnetic materials, which can offer insights into the influence of the magnetic state on the behavior of nuclear fuels at high temperatures.

We have no conflicts of interest to disclose.

Thank you for your consideration of this manuscript.

Sincerely,

Benjamin Beeler