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Dear Journal of Nuclear Materials,

On behalf of my co-authors and myself, I am hereby submitting our manuscript, entitled ``*Ab initio molecular dynamics investigation of point defects in gamma-U*”, for publication in the *Journal of Nuclear Materials*.

This article provides the first ab initio molecular dynamics investigation of point defects in gamma U, which had previously only been performed at 0 K with traditional DFT, producing somewhat anomalous results. This work provides a very strong basis for the existence of very low interstitial formation energies in gamma U, and for self-diffusion occurring via an interstitialcy mechanism. The development of large-scale high-performance computing machines are now allowing for studies such as this to be performed, which were previously deemed far too computationally expensive.

In addition to defect formation energies, the diffusion coefficients, thermal expansion, heat capacity and bulk modulus are determined for gamma U as a function of temperature. This work compares favorably to experiment, and provides insights into defect behavior with a greater degree of scientific rigor than was previously achievable.

We feel this work greatly adds to the scientific community and provides a starting point for rapid advancement in the deployment of AIMD to study nuclear fuels.

Sincerely,

Benjamin Beeler