Cover letter

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Dear Sir or Madam,

We wish to submit an original research article entitled “Assessment of uranium nitride interatomic potentials” for consideration by the Journal of Nuclear Materials.
We confirm that this work is original and has not been published elsewhere, nor is it currently under consideration for publication elsewhere.

Uranium mononitride (UN) is a promising nuclear fuel due to its high fissile density, high thermal conductivity, and suitability for reprocessing. In this study, two uranium nitride interatomic potentials are assessed: Tseplyaev and Starikov's angular-dependent potential and Kocevski *et al*.'s embedded atom model potential. Predictions of the thermophysical and elastic properties of UN, UN_2, and α- and β-U_2N_3 computed using both potentials are assessed and compared to available experimental data. The Tseplyaev potential performs better with the energetic aspects of perfect UN, e.g., specific heat capacity and point defect formation energies, whereas the Kocevski potential performs better with the structural aspects of perfect UN, e.g., thermal expansion and elastic properties. The reasons why the Kocevski potential underestimates the UN specific heat are explained by examining the UN phonon properties modeled using both potentials. The Kocevski potential shows better identification of the mechanical stability ranges of UN, UN_2, and α- and β-U_2N_3, reasonably predicting the melting point of UN and predicting stable structures for UN_2 and α- and β-U_2N_3. On the other hand, the Tseplyaev potential predicts a premature phase change of both UN and UN_2 and cannot stabilize α- nor β-U_2N_3. However, the Kocevski potential cannot predict a stable α-U phase and is thus not suitable for the calculation of formation energies for non-stoichiometric point defects.

We have no conflicts of interest to disclose.

Please address all correspondence concerning this manuscript to bwbeeler@ncsu.edu.

Thank you for your consideration of this manuscript.

Sincerely,

Mohamed AbdulHameed