Contribution ID: **33** Type: **poster**

Benchmarking foundation models for simulating radiation damage in iron alloys

Machine-learned interatomic potentials (MLIPs) are a promising new approach that allow us to make atomistic material predictions with close to first principles DFT accuracy at a fraction of the cost. The new developments of foundation model MLIPs over the last year [1,2] are especially promising for modelling alloys. In this poster, I will benchmark an iron MLIP that we have developed using the atomic cluster expansion framework, as well as two new foundation models from the literature (MACE-MP [1] and GRACE [2]), for modelling of typical high energy environments generated in collision cascade simulations of iron. This will help identify areas of improvement to apply these MLIPs for primary radiation damage modelling. I will also benchmark the point defect and solute migration barriers predicted by the foundation models for RAFM steel alloy compositions, and test the possibility of improving their accuracy via fine-tuning. The goal of the latter benchmark is to work towards providing higher accuracy inputs from such atomistic calculations to larger-scale models of irradiation-induced microstructure evolution in steel.

References:
1. Batatia, Ilyes, et al. "A foundation model for atomistic materials chemistry." arXiv preprint arXiv:2401.00096 (2023).
2. Bochkarev, Anton, Yury Lysogorskiy, and Ralf Drautz. "Graph atomic cluster expansion for semilocal interactions beyond equivariant message passing." Physical Review X 14.2 (2024): 021036.

Primary author: SHENOY, Lakshmi (University of Sheffield)

Presenter: SHENOY, Lakshmi (University of Sheffield)