# SuperSalts: Equivariant Neural Network Force Fields for Multicomponent Molten Salts System

Chen Shen[1*†], Siamak Attarian[1†], Yixuan Zhang[2], Hongbin Zhang[2], Mark Asta[3], Izabela Szlufarska[1], Dane Morgan[1*]

[1*]Materials Science and Engineering, University of Wisconsin-Madison, Madison, 53706, Wisconsin, United States.

[2*]Materials Science, Technical University of Darmstadt, Darmstadt, 64287, Hessen, Germany.

[3*]Materials Science and Engineering, University of California, Berkeley, 94720, California, United States.

*Corresponding author(s). E-mail(s): cshen89@wisc.edu; ddmorgan@wisc.edu;
Contributing authors: sattarian@wisc.edu; yixuan.zhang@tu-darmstadt.de; hzhang@tmm.tu-darmstadt.de; mdasta@berkeley.edu; szlufarska@wisc.edu;
†These authors contributed equally to this work.

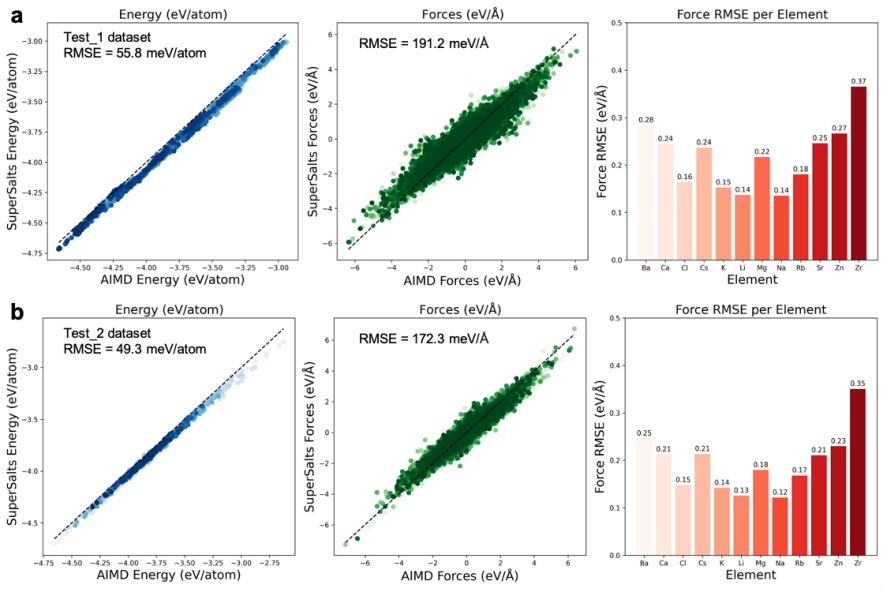


**Fig. S1**: Parity plots for energy and force, comparing DFT reference data with MACE-MP0 potential predictions, are shown for (a) Test_1 containing the 3300-ternary dataset, and (b) Test_2 containing the 800-multicomponent dataset. The corresponding force RMSE per element for each dataset is presented as histograms in the third column.

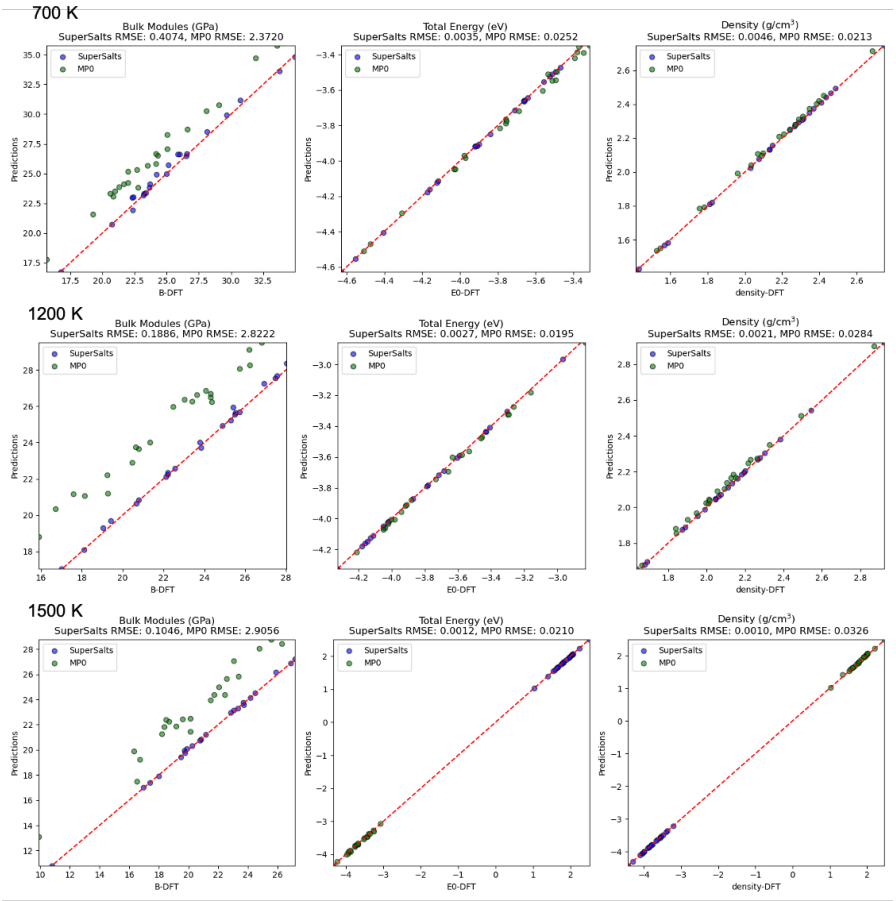


**Fig. S2**: Parity plots for bulk modules, total energies, and densities, comparing DFT reference data with SuperSalt and MACE-MP0 potential predictions at different temperatures.