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Sampling Models for Machine Learned Atomistic Potentials - The Case of Water AMBER MAHARAJ, University of Ontario, Institute of Technology, ISAAC TAMBLYN, University of Ontario, Institute of Technology, National Research Council of Canada — Computational restrictions on system size and accessible time scales in atomistic simulations inhibit the investigation of mesoscopic materials. While *ab initio* methods provide accurate energies and forces, they are unable to efficiently sample configuration space. Classical force fields and semi empirical methods give an efficient sampling of configuration space, but with weights and energies that differ from *ab initio* methods. Here we consider the relationship between the optimal configurational sampling method and electronic structure approach for calculating total energies and forces (for the particular case of water) of a liquid. Using the Atomic Energy Network (aenet) approach, we apply machine learning to the generation of interaction potentials of water models such as TIP3P, TIP4P and TIP5P, and reference data from DFTB, and DFT. The use of machine learned potentials reduces the algorithmic complexity of simulations while achieving accuracy comparable to *ab initio* methods. To verify the accuracy of the generated potentials, physically observable quantities are computed and compared to *ab initio* and experimental data.

Amber Maharaj
Univ of Ontario

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