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Machine learning models of many-body atomic and electronic interactions

To advance the capability of density functional theory (DFT) we introduce non-local charge density descriptors that satisfy exact scaling constraints and learn exchange functionals called CIDER, that are orders of magnitude faster to evaluate than hybrid functionals but similar in accuracy [1]. To accelerate molecular dynamics, we use machine learning to capture the potential energy surfaces obtained from quantum calculations. We developed NequIP [2] and Allegro [3], the first deep equivariant neural network interatomic potential models, whose symmetry-preserving layer architecture achieves state-of-the-art data efficiency and accuracy for simulating dynamics. To enable autonomous active learning of reactive systems, we developed the FLARE [4] algorithm that constructs accurate and uncertainty-aware Bayesian force fields on-the-fly from a molecular dynamics simulation, using Gaussian process regression.

[1] K. Bystrom, B. Kozinsky, arXiv:2303.00682 (2023)

[2] S. Batzner et al, Nature Comm. 13 (1), 2453 (2022)

[3] A. Musaelian, S. Batzner et al, Nature Comm. 14, 579 (2023)

[4] J. Vandermause et al, Nature Comm. 13 (1), 5183 (2022)