

LiFlow for amorphous structures: initial experiment

■ Amorphous LPS simulation settings

- 250 ps trajectory from [Jun et al., 2024], amorphous Li_3PS_4 @ 800 K, 1.8 g/cm^3 (128 atoms); first 50 ps for training
- Propagator scales 10.0 (Li), 2.5 (frame), Corrector noise scale 0.2
- Slower convergence of Propagator when the system is amorphous \rightarrow Propagator trained for 200k steps

■ Observations

- Dynamics: Slightly lower diffusivity (AIMD $4.33 \times 10^{-5} \text{ cm}^2/\text{s}$ vs. LiFlow $3.88 \times 10^{-5} \text{ cm}^2/\text{s}$)
- Static features: RDFs are well reproduced overall, with less structured long-range Li-Li and Li-P interactions

