# Transferable Boltzmann Generators

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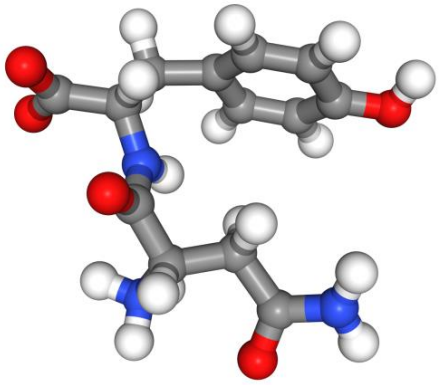
# Motivation – the Sampling Problem



- Generate equilibrium samples from Boltzmann distributions

$$\mu(x) \propto \exp\{-u(x)\}$$

- Molecular Dynamics can be inefficient as samples are correlated
- Boltzmann Generators produce independent sample

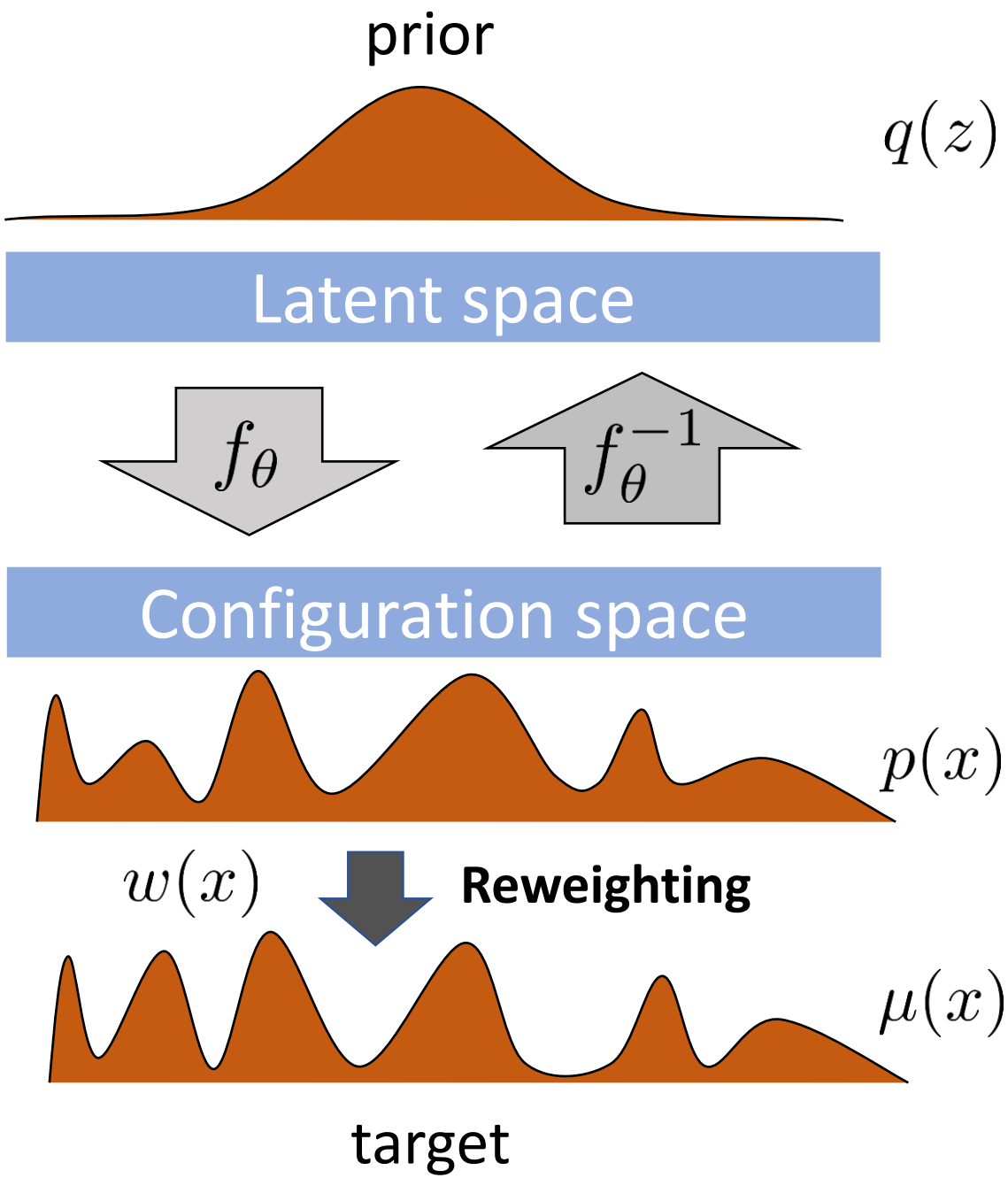
→ First *transferable* Boltzmann Generator

# Boltzmann Generators

Sampling:

1. Sample from prior $z \sim q(z)$
2. Transform sample $x = f_\theta(z)$
3. Reweight wrt target distribution

$$w(x) \propto \frac{\mu(x)}{p(x)}$$




[1] F. Noé, S. Olsson, J. Köhler, and H. Wu. Boltzmann generators-sampling equilibrium states of many-body systems with deep learning. *Science*, 365:eaaw1147, 2019.

# Continuous normalizing flows

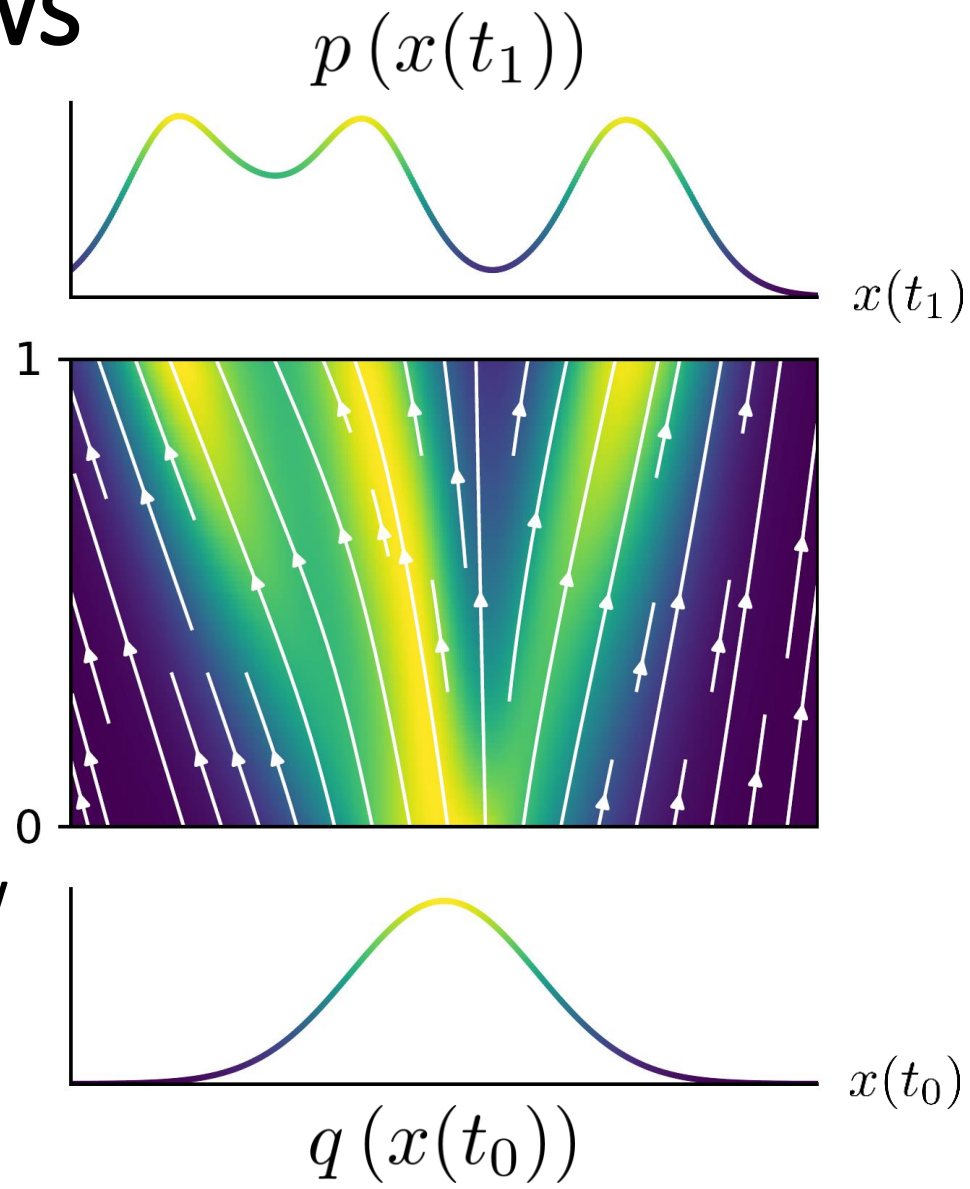
- Solve initial value problem of ODE

$$\frac{dx(t)}{dt} = v_\theta(x(t), t), \quad x_0 = x(t_0)$$

- Invertible transformation

$$x(t_1) = f_\theta(x(t_0)) = x(t_0) + \int_{t_0}^{t_1} dt\ v_\theta(x(t), t)$$

- Equivariant vector field → equivariant flow

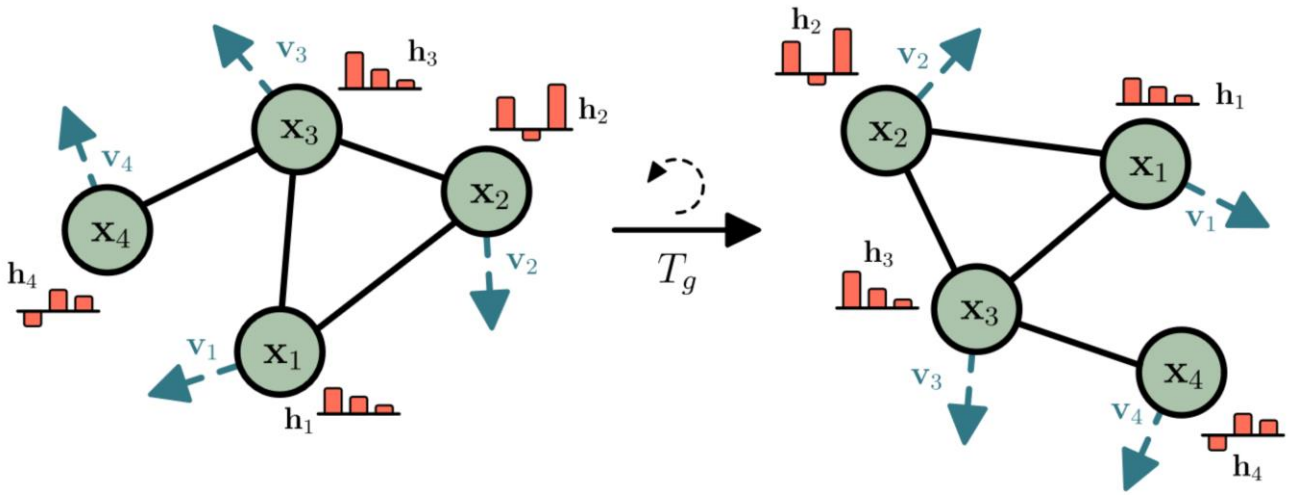



[2] Tian Qi Chen et al. Neural ordinary differential equations. *NeurIPS*, 2018.
Figure: [3] W. Grathwohl et al. FFJORD. *ICLR*, 2019.

# Equivariant network architecture

**Equivariant graph neural network (EGNN)**

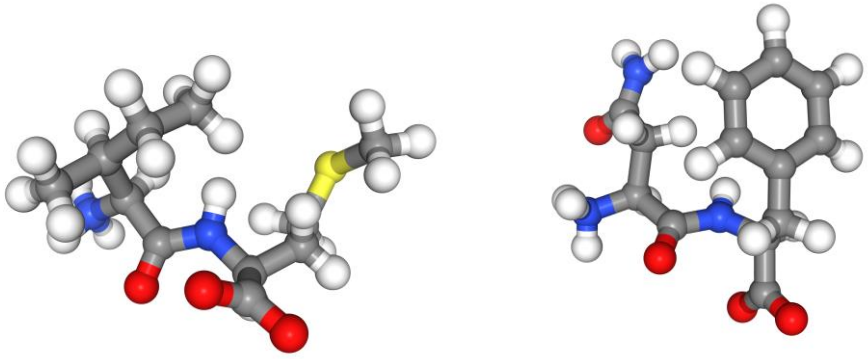
+ Desired equivariances
  - Permutations of same atom type
  - Global rotations
+ Fast evaluation
+ Expressive
+ Transferable




[4] Vıctor Garcia Satorras, Emiel Hoogeboom, and Max Welling. E(n) equivariant graph neural network. *ICML* 2021

# Dipeptides

- Classical force field
- 200 train dipeptides
- 100 test dipeptides



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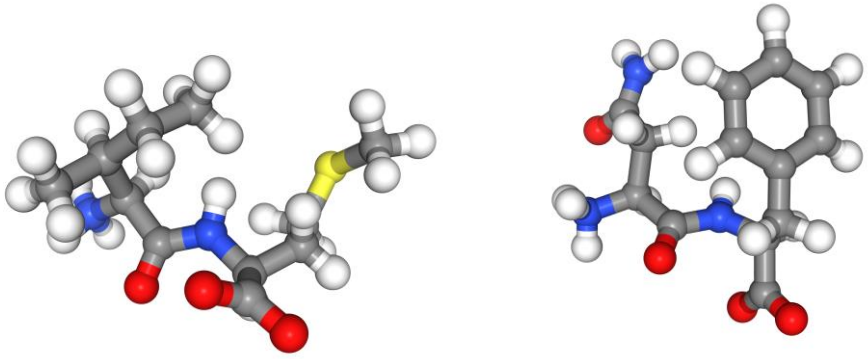
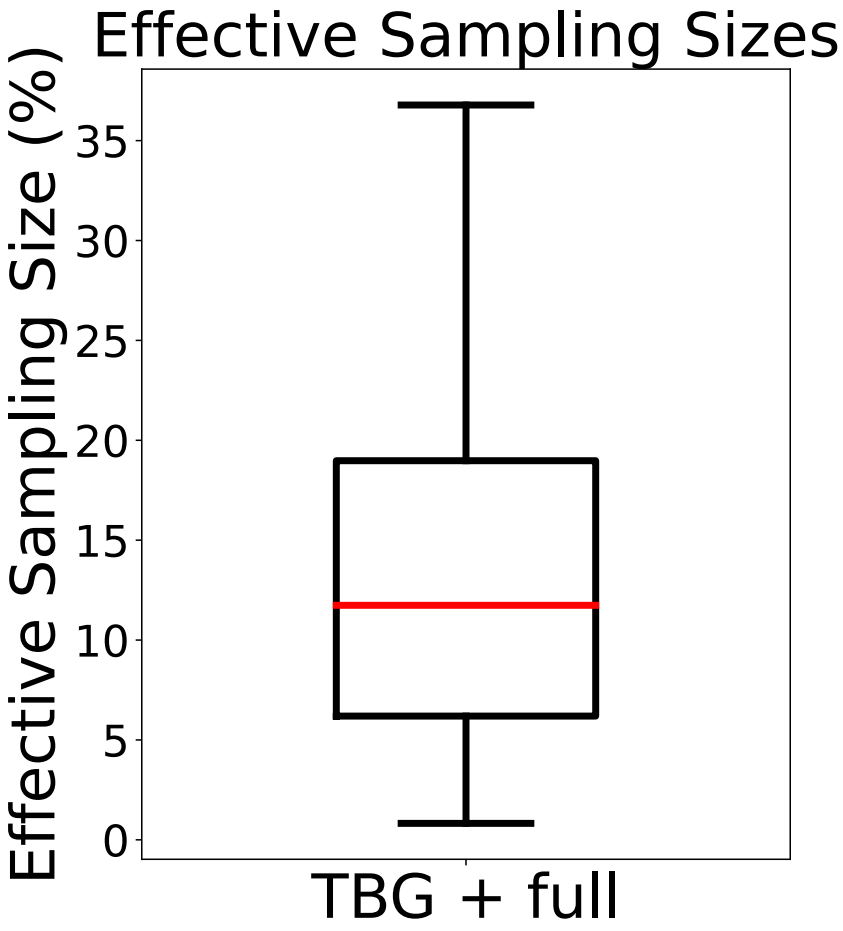
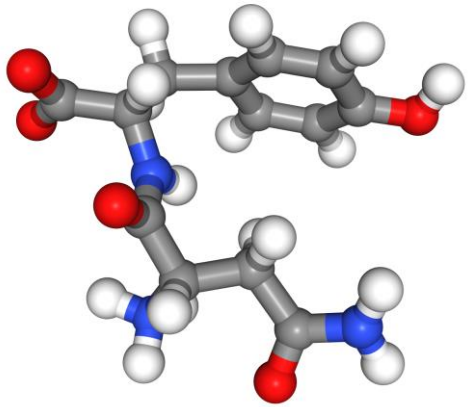
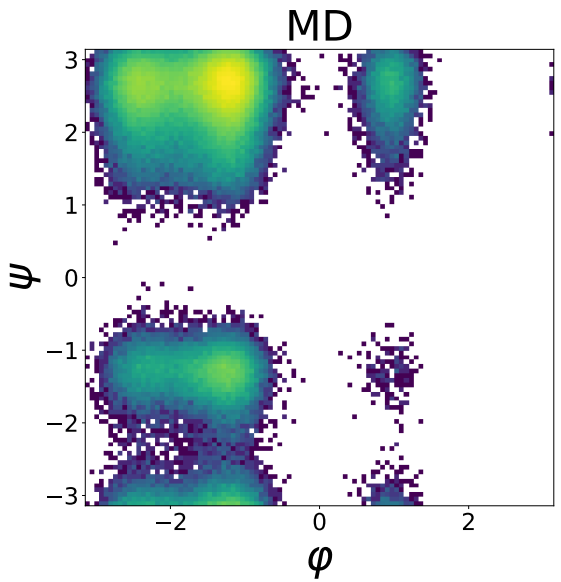
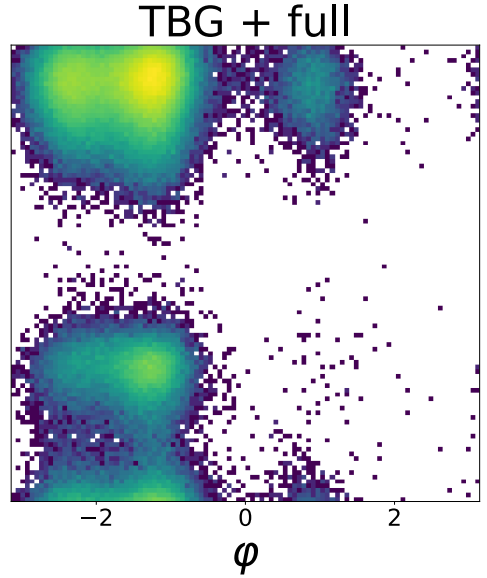




# Dipeptide NY (ESS = 10%)





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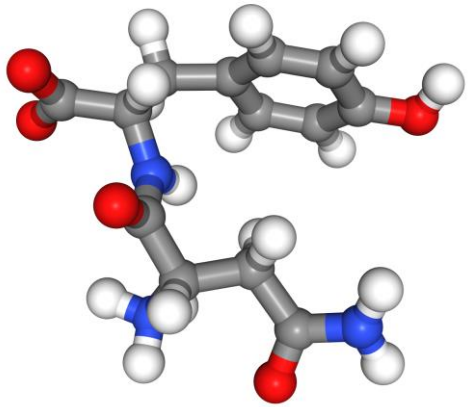

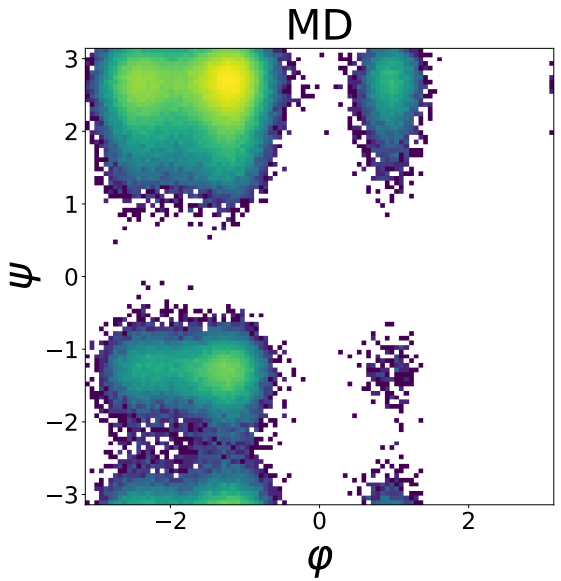


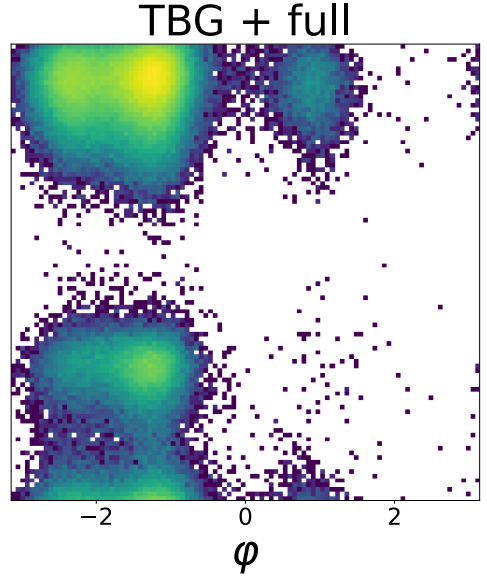


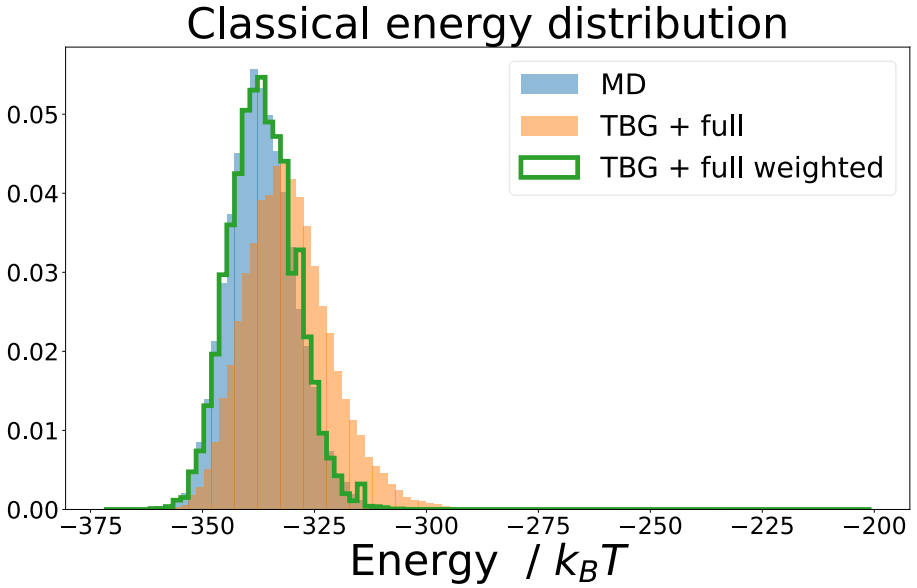


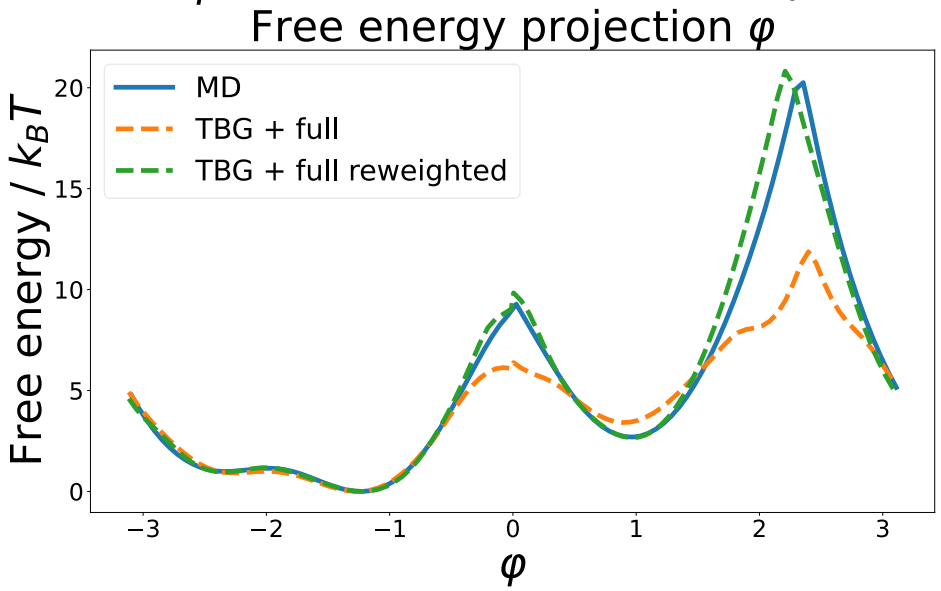

# Thank you for listening