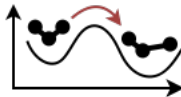


(a)*valid structures**denoising objective**learned GNN encoder* h_i **(b)***molecular simulations**frozen GNN encoder**geometric features***(c)***frame features* X_0  X_t *downstream tasks**committor, VAMPnet**dynamical information* $tIC\ 2$  $tIC\ 1$