a

$T \longleftarrow t \longrightarrow 0$ *axis of time*

Equivariant Single Molecule Diffusion

ϵ_t ϵ_0

$z_T = \mathcal{N}(0,1)$ z_t z_0

$\hat{\epsilon}_\theta^{SE(3)}(z_T, T)$ $\hat{\epsilon}_\theta^{SE(3)}(z_t, t)$

b

Object-Aware Equivariant Elementary Reaction Diffusion

$\hat{\epsilon}_\theta^{OA-SE(3)}(z_T, T)$ $\tilde{z}_t^{R,P} = \tilde{z}_{t,R} \times z_{t,TS} \times \tilde{z}_{t,P}$ $\hat{\epsilon}_\theta^{OA-SE(3)}(\tilde{z}_t^{R,P}, t)$

Inpainting

$\tilde{z}_{t,R}$ ϵ_0 ϵ_0

ϵ_t $\tilde{z}_{t,P}$ ϵ_0

$z_T = \mathcal{N}(0,1) \times \mathcal{N}(0,1) \times \mathcal{N}(0,1)$ $z_t = z_{t,R} \times z_{t,TS} \times z_{t,P}$ $z_0 = z_{0,R} \times z_{0,TS} \times z_{0,P}$

unconditional
generation $\hat{\epsilon}_\theta^{OA-SE(3)}(z_T, T)$ $\hat{\epsilon}_\theta^{OA-SE(3)}(z_t, t)$
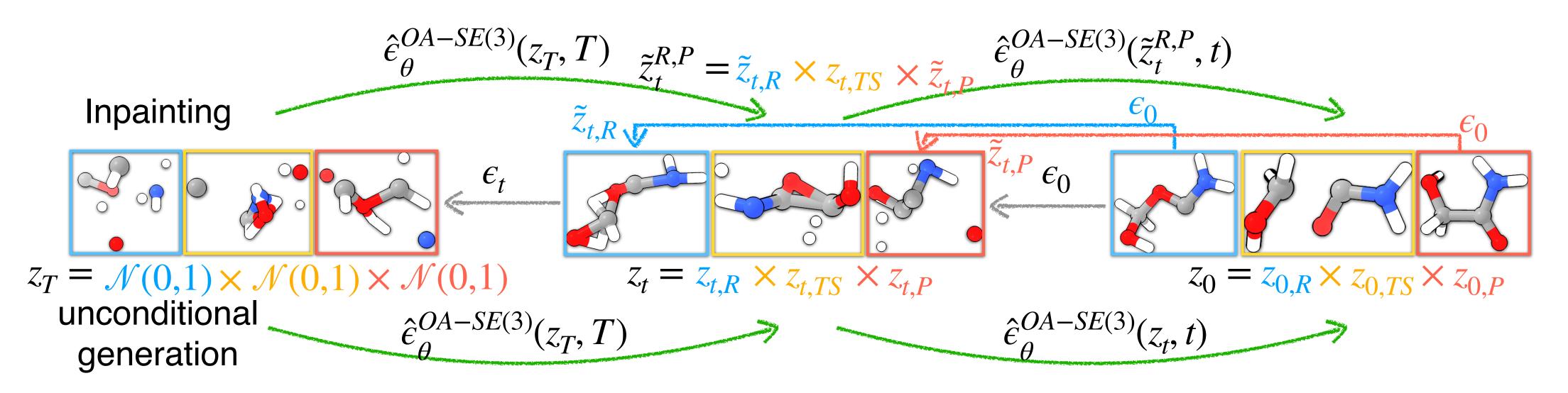
ϵ : diffuse $\hat{\epsilon}_\theta$: denoise z : data representation t : time frame