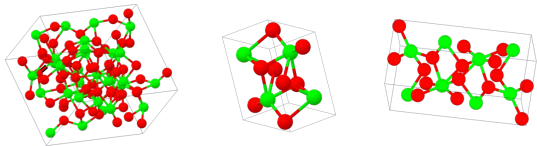


ZrO₂

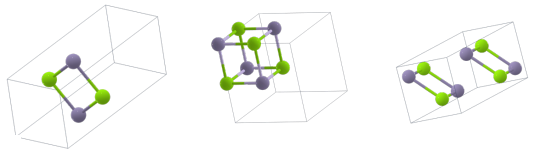
Polymorphic structures (\mathcal{P}^a)



f^b



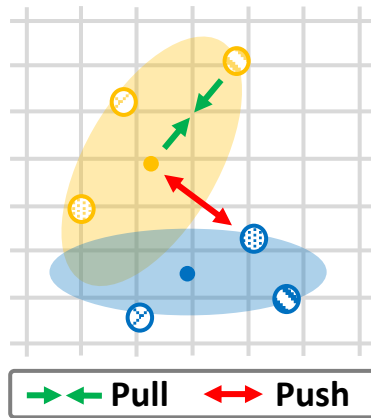
SnSe



f^b



Structural Graph Encoder



Representation space

z_μ^a

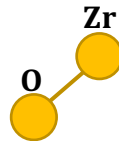
f_μ^a

z_σ^a

f_σ^a

Z^a

f^a



ZrO₂

z_μ^a

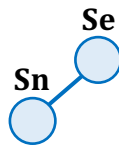
f_μ^a

z_σ^a

f_σ^a

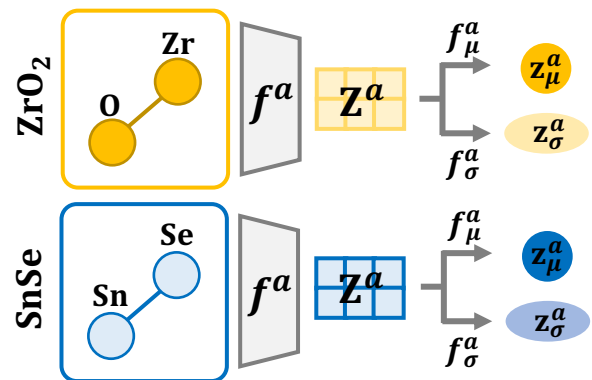
Z^a

f^a

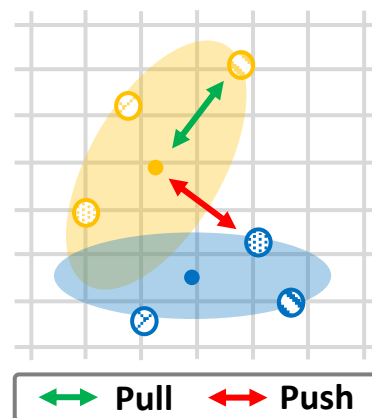


SnSe

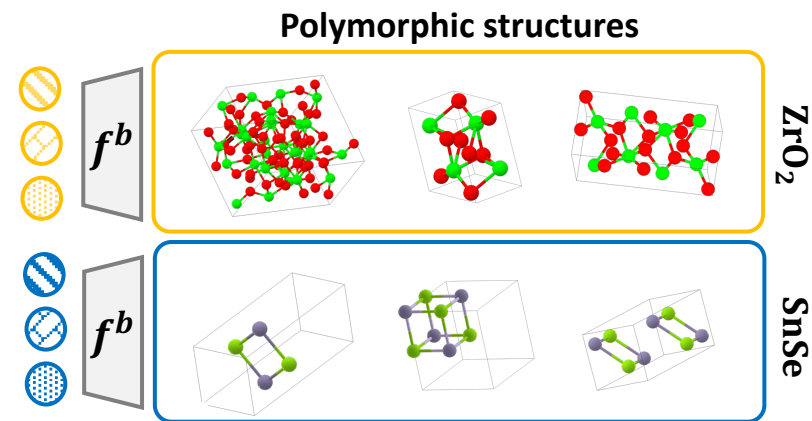
Probabilistic Composition Encoder



Probabilistic Stoichiometry Encoder



Representation space



Structural Graph Encoder