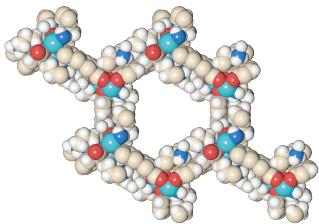
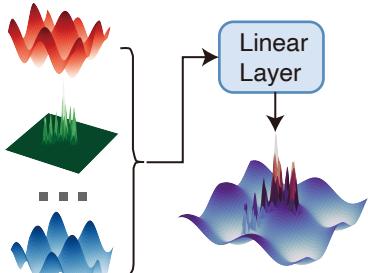


## Descriptors

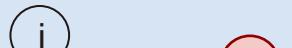


Material Structure



Potential Energy Surface Basis Function

## Model Architecture



Graph Neural Network

Cross Attention

Transformer

CLS

Vision Transformer

$F_1$

$F_2$

$\dots$

$F_x$

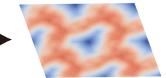
CLS

Downstream Head

## Pre-training

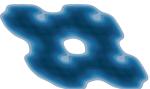
Atomic-level

SDF Head



Signed Distance Function

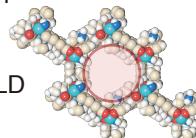
ANP Head



Number of Atoms

Material-level

Topo Head



PLD Head

LCD, Void Fraction...

## Downstream Tasks

### Properties Related to Guest Molecules

- Gas Uptake
- Henry's Constant
- Gas Separation
- Adsorption Heat
- Gas Diffusion

### Intrinsic Properties

- Thermo Stability
- Elastic Modulus
- Heat Capacity
- Shear Modulus

### Out-of-distribution Materials

- Covalent organic frameworks (COFs)
- Zeolites
- Porous polymer networks (PPNs)