MESSAGE PASSING NEURAL NETWORKS TO PREDICT ADSORPTION PROPERTIES OF NANOPOROUS MATERIALS

An Application of Graph Neural Networks

DISCOVERING MATERIALS FOR GAS STORAGE AND SEPARATION

Covalent Organic Frameworks (COFs)

- Assembled modularly from organic molecules through strong covalent bonds.
- 560,000 discrete structures hypothesized computationally to date.
- Exceptional porosity affords exemplary storage and separation of gasses.
- Applications include carbon capture, low pressure fuel storage, cancer detection, etc.

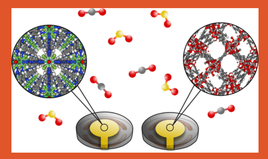

Fig 1. Gravimetric Gas Array Sensors using MOFs

TOOLS & PITFALLS IN COMPUTATIONAL CHEMISTRY

The adsorption properties of most COFs are unknown. **How do we know which are best suited for our application?**

- **Synthesis:** COFs can be synthesized and tested, but this is costly and inefficient.
- **Simulations:** Molecular dynamics are extremely accurate, but also computationally expensive.
- **Machine Learning:** Has the potential to be very accurate and efficient, but often relies on hand-crafted features as inputs, which are not readily available.

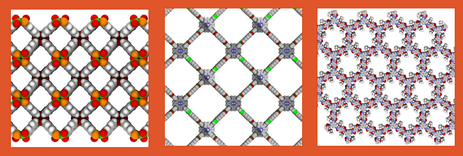

Fig 2. Various crystal structures of COFs

MATRIX FACTORIZATION & THE COLD START

An innovative approach to learning adsorption properties is the recommender system approach.

- Learns to predict adsorption by observing a partially complete target-set, overcoming the need for hand crafted features. However, each material requires 1 or more known targets to compute.

How do we approach a cold start problem, in which no targets, and only the molecular structure is known?

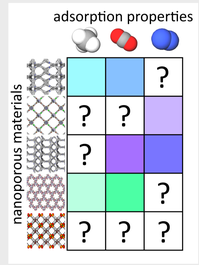

Fig 3. An incomplete material-property matrix with the cold-start problem

MESSAGE PASSING NEURAL NETWORKS (MPNNS)

We design and train an MPNN to predict uptakes of 16 different gasses. We train on a partially complete set of adsorption tasks (Θ) and the molecular graph. **Our model only requires the molecular graph as input during inference, thus overcoming the cold start problem.**

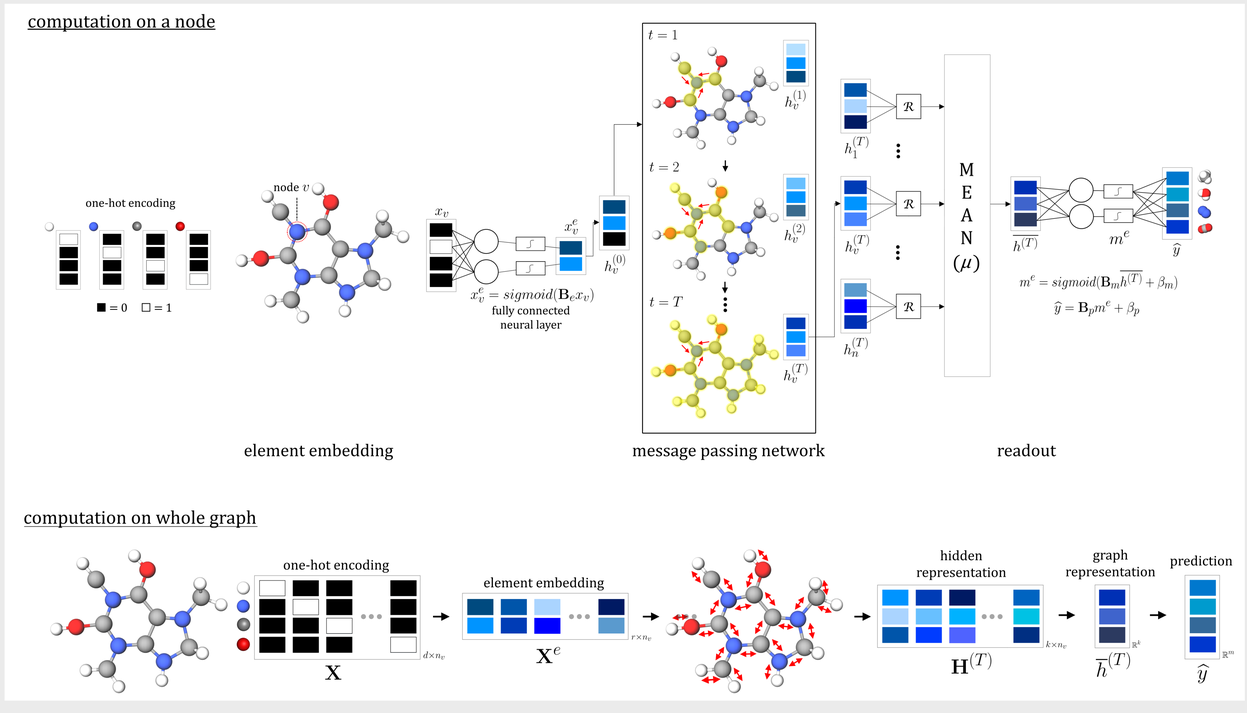

Fig 4. Our MPNN Architecture, which learns a vector representation of the COF m^e that is then used to generate prediction $\hat{y}$

Learn More!

GRAPH SIMILARITY

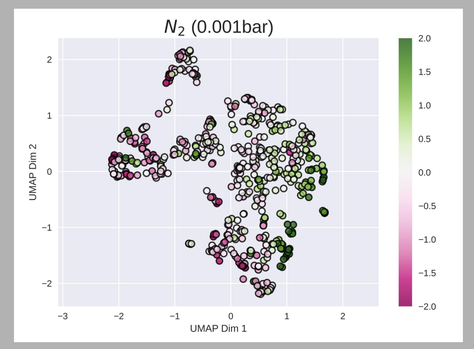

Fig 5. UMAP where each point represents a COF colored by its N_2 adsorption.

We find that the learned vector representation m^e correlates well to adsorption tasks, seen by the clusters of COFs with similar uptake in *Fig 5*.

MODEL PERFORMANCE

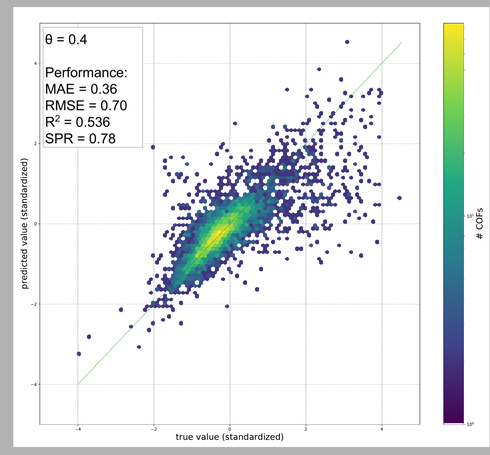

Fig 6. Parity plot mapping all predicted vs actual adsorption tasks

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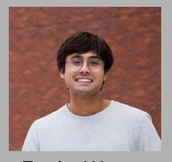
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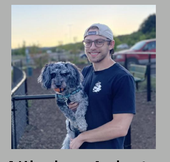
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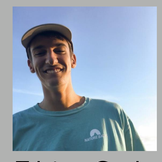
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