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Graph Representation Learning & Deep Generative Models On Graphs

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Content

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1. Graph representation learning:
   - Message passing neural networks
   - Permutation equivariance
   - Covariant compositional networks
2. Deep generative models on graphs:
   - Variational Autoencoder
   - Equivariant graph/molecule generation

Message passing neural networks

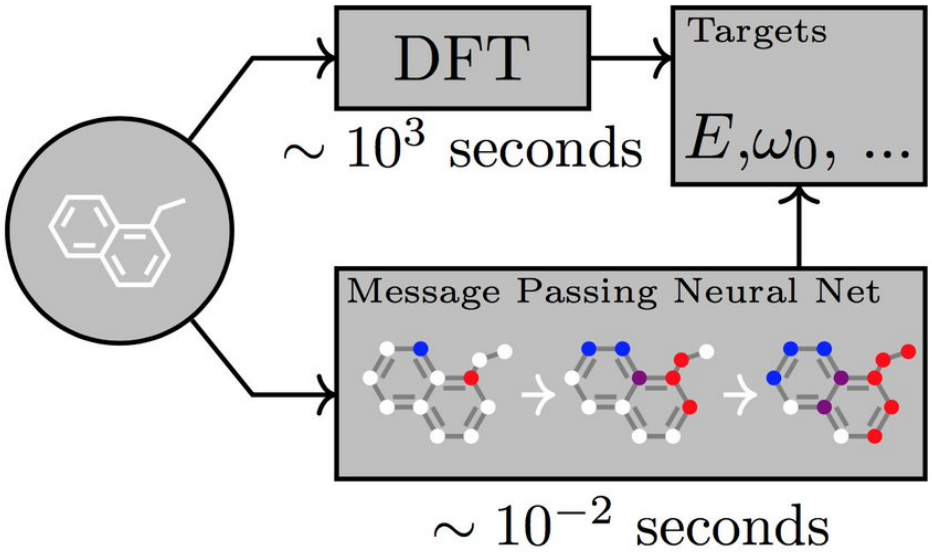
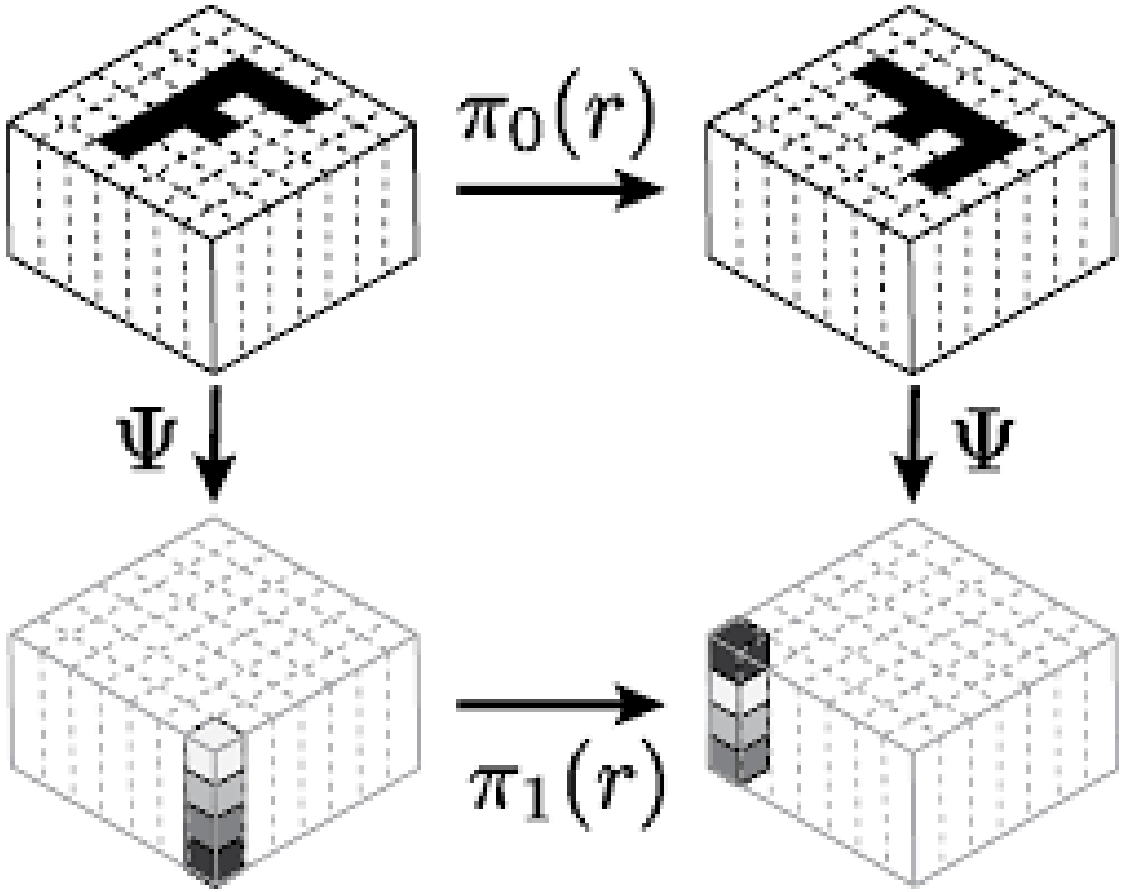


Figure 1. A Message Passing Neural Network predicts quantum properties of an organic molecule by modeling a computationally expensive DFT calculation.

Neural Message Passing for Quantum Chemistry, ICML 2017

Equivariance



Steerable CNNs, Taco S. Cohen, Max Welling,
https://arxiv.org/abs/1612.08498

Permutation equivariance on graphs (1)

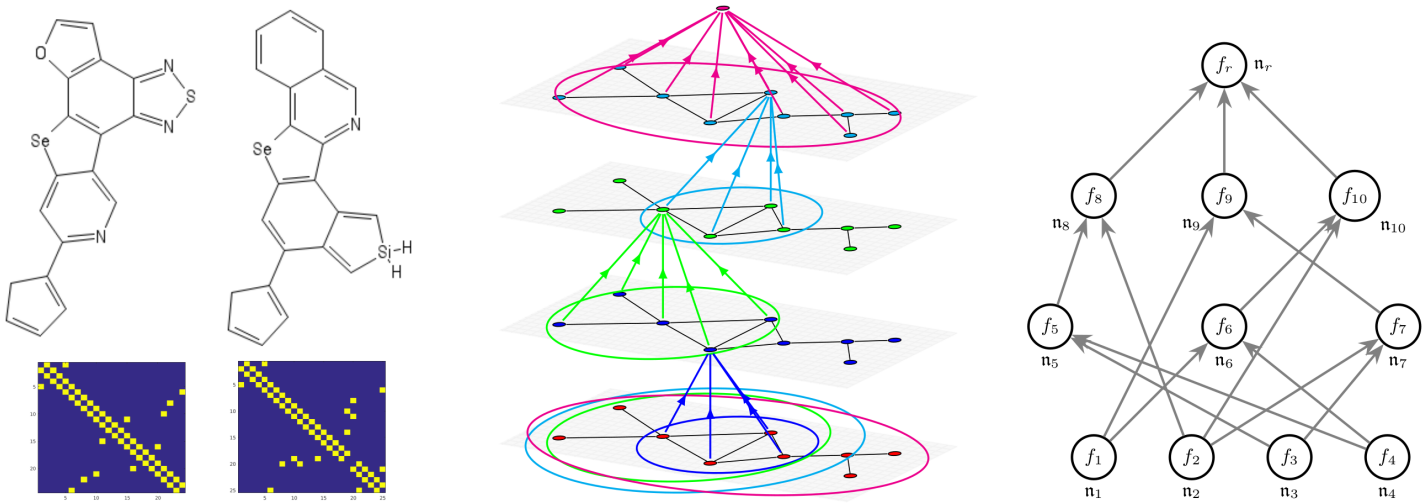
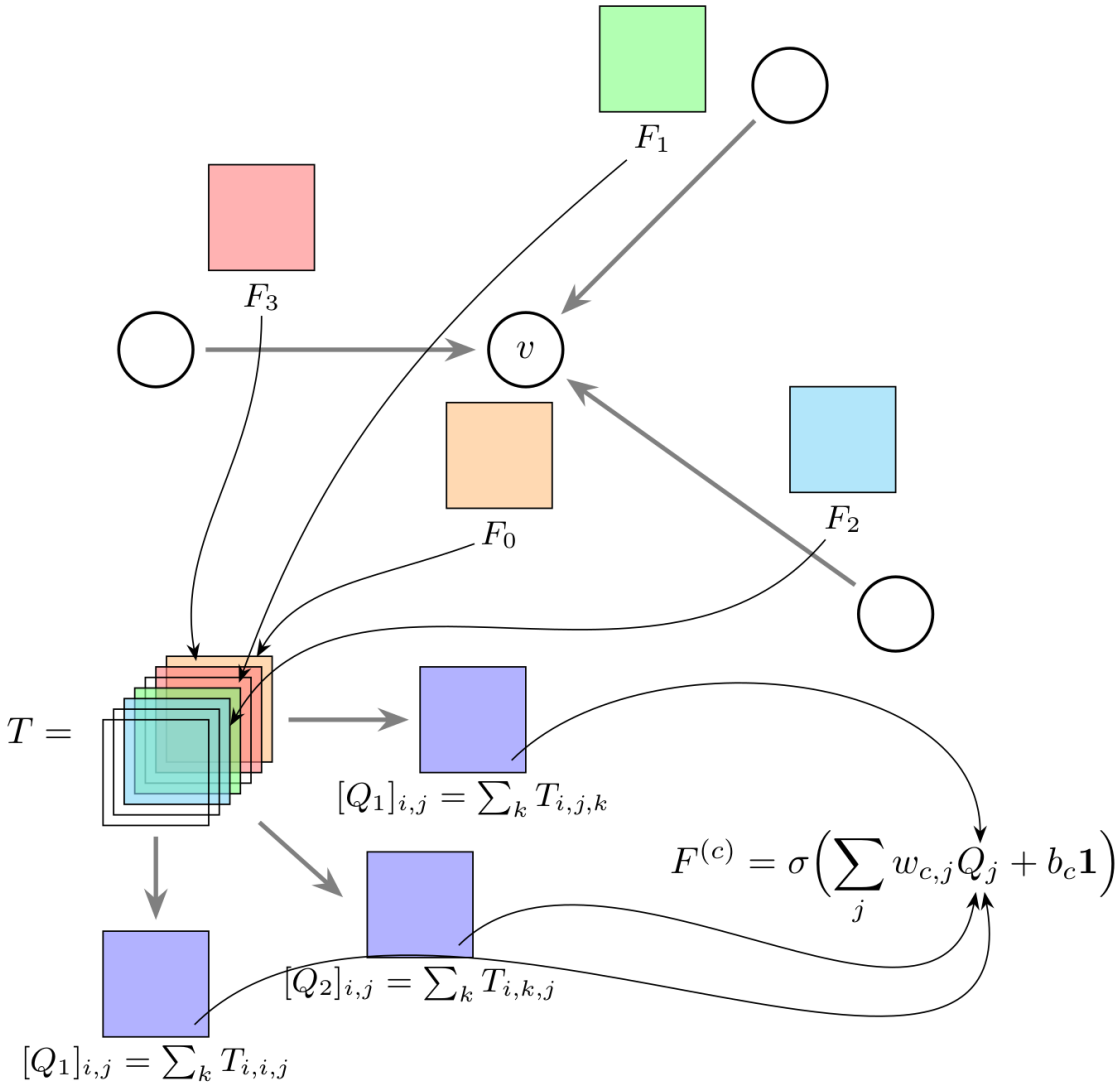


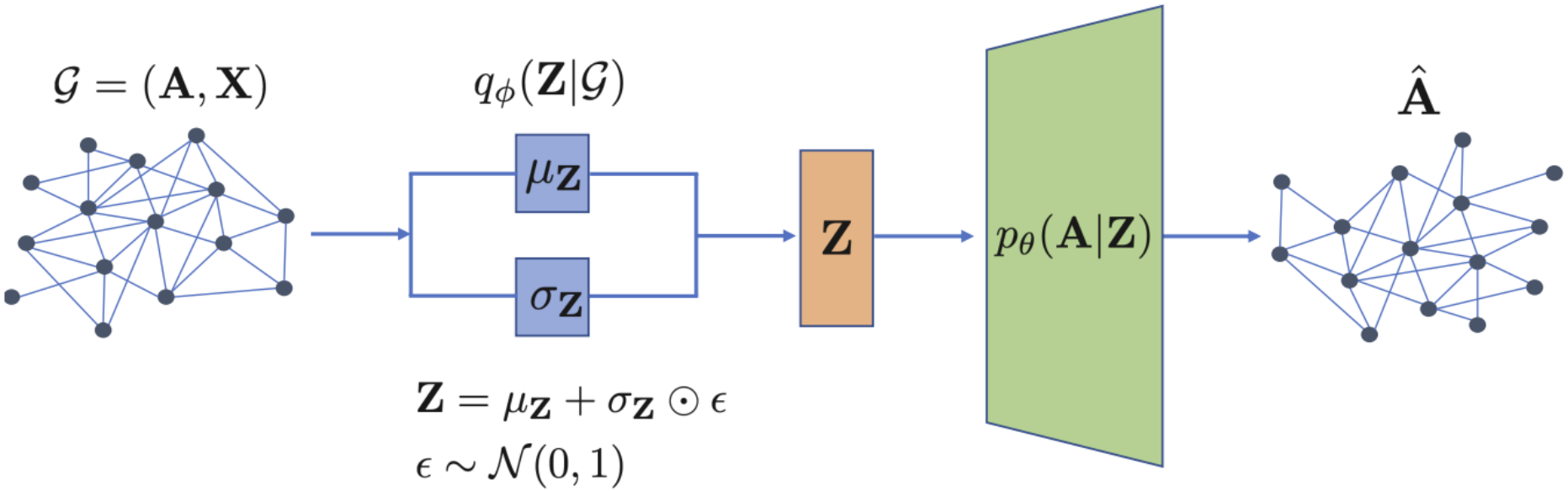
FIG. 1. **Left:** Molecular graphs for $C_{18}H_9N_3OSSe$ and $C_{22}H_{15}NSeSi$ from the Harvard Clean Enery Project (HCEP)[4] dataset with corresponding adjacency matrices. **Center and right:** The comp-net of a graph $\mathcal{G}$ is constructed by decomposing $\mathcal{G}$ into a hierarchy of subgraphs $\{\mathcal{P}_i\}$ and forming a neural network $\mathcal{N}$ in which each "neuron" $\mathfrak{n}_i$ corresponds to one of the $\mathcal{P}_i$ subgraphs, and receives inputs from other neurons that correspond to smaller subgraphs contained in $\mathcal{P}_i$. The center pane shows how this can equivalently be thought of as an algorithm in which each vertex of $\mathcal{G}$ receives and aggregates messages from its neighbors. To keep the figure simple, we only marked aggregation at a single vertex in each round (layer).

Predicting molecular properties with covariant compositional networks, https://aip.scitation.org/doi/10.1063/1.5024797

Permutation equivariance on graphs (2)



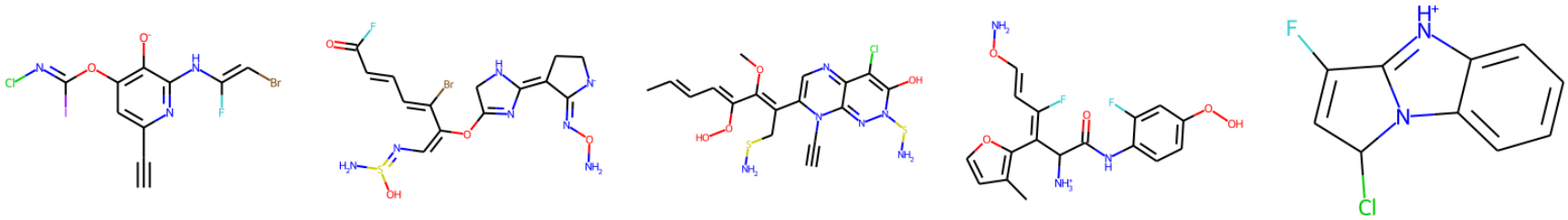
Variational Autoencoder



Graph Representation Learning, William L. Hamilton (McGill University, 2020) `https://www.cs.mcgill.ca/~wlh/grl_book/`

Equivariant molecule generation

Generated examples (model trained on ZINC):



Interpolation on the latent: