VIDY Reading Group
3-D Molecule: SchNet & SphereNet

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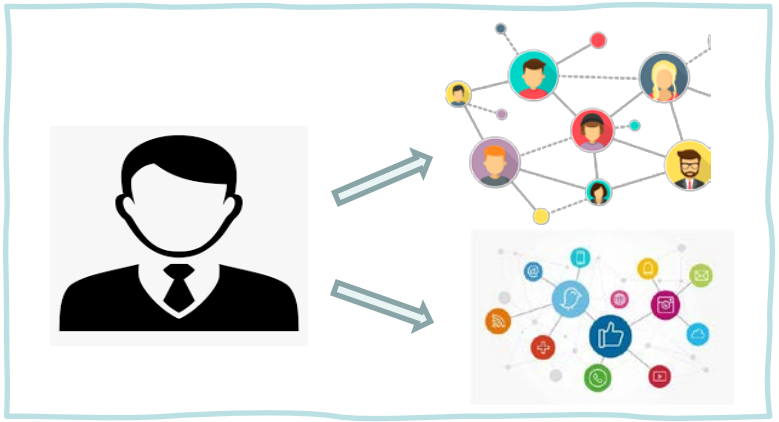
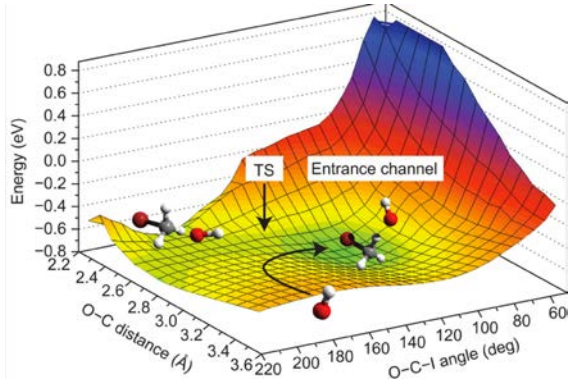
About Me

- My previous works mainly focus on **unsupervised multi-view graph clustering**, wherein six works are proposed to extract structural **consensus** and **completeness** inherent in different graphs by proposing the techniques of **pseudo-label self-supervision** (ICONIP), **graph refinement** (AAAI), **graph generation** (under review), **heterophilous graph mining** (AAAI), etc.
- Currently, my research interests primarily lie in the realm of **3D graph** modeling, particularly its application in 3D molecules, such as **molecular dynamic simulation** and 3D GNN for **material design**, etc.

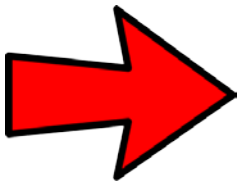


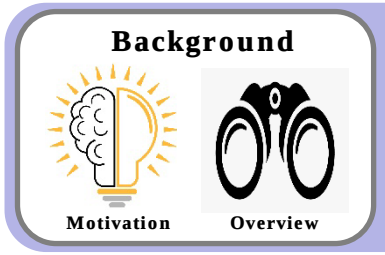
Multi-View Graph Clustering
Identify a person from their social network and interaction network.



Potential Energy Prediction
molecular dynamic simulation via PES prediction

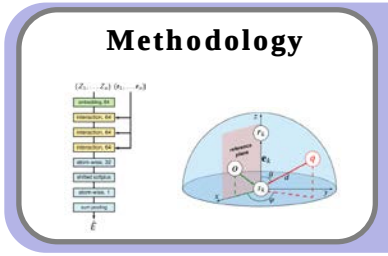
Roadmap





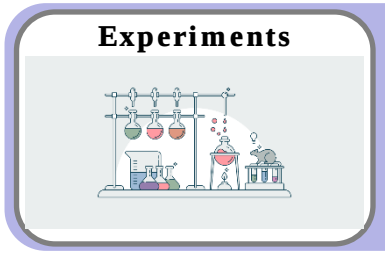
I. Background

- Molecular graph modeling
- 3D Graph



II. Spherical Message Passing for 3D Molecular Graphs

- Background & Motivation
- Spherical Message Passing Scheme & Completeness
- SphereNet



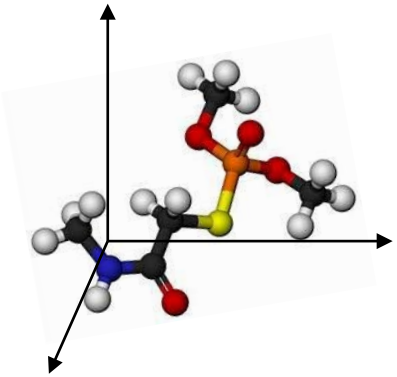
III. Experiments & Analysis

- Ablation Study
- Completeness VS Efficiency

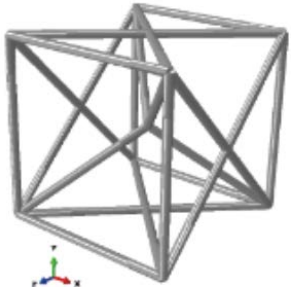
IV. Conclusion

Background

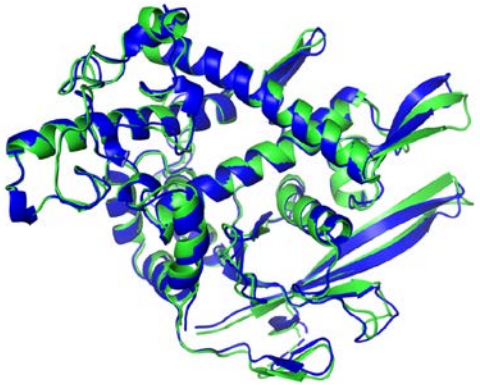
❑Molecular graphs: Applications



Small molecules
=> Property predictions



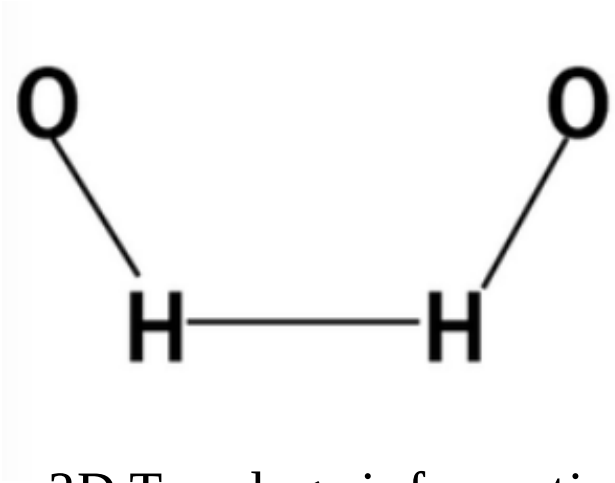
Crystals
=> Material design



Proteins
=> Protein discovery

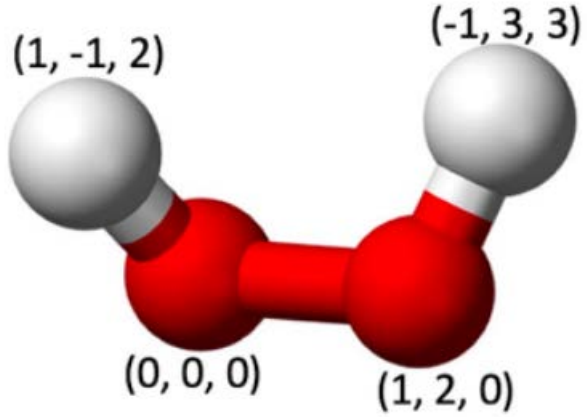
Background

❑ **Molecules as graphs:**



2D Topology information

Basic information, only contains connectivity.



3D Position information

Identify a conformation.

3D graph: 3D **coordinates** & **Connectivity** information

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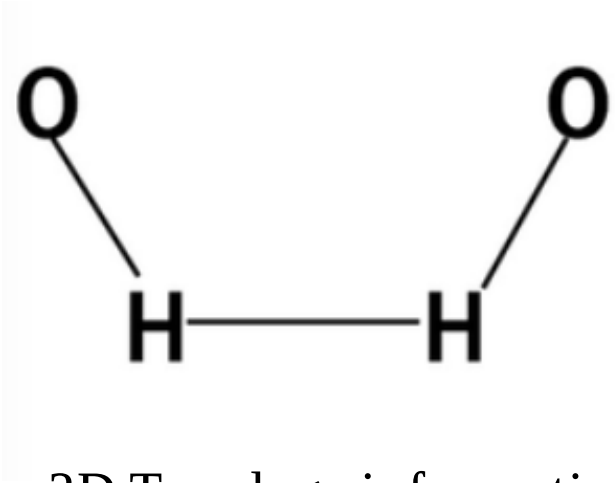

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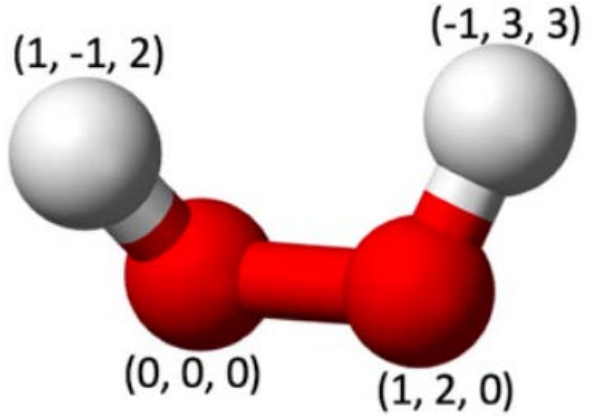

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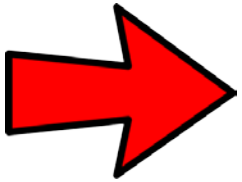
3D graph: 3D **coordinates** & **Connectivity** information

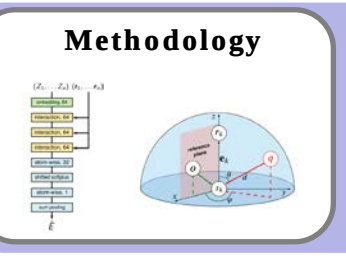
How to conduct message passing on 3D graphs?

Roadmap



I. Background

- Message Passing Scheme
- 3D Graph



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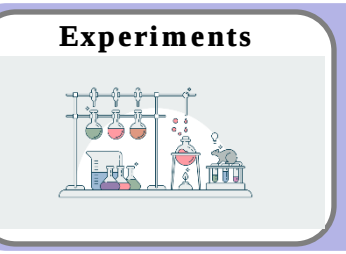

III. Experiments & Analysis

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Background: Equivariant & Invariant

- 3D graph GNNs: SE(3) **Equivariant** & **Invariant** to translations and rotations.

Equivariant

The prediction will be **transformed** according to the transformation of input graph.

$$f(g \cdot x) = r(g) \cdot f(x)$$

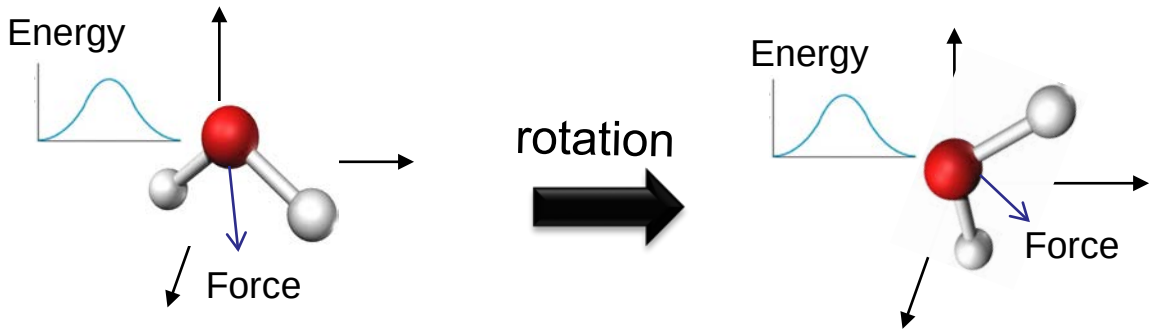
Example: Force direction

Invariant

The prediction will stay **unchanged** regardless of the SE(3) transformation of input graph.

$$f(g \cdot x) = f(x)$$

Example: Graph energy

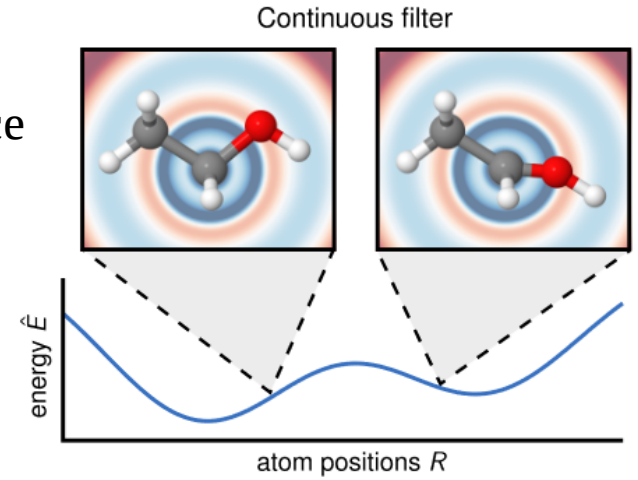


Background: Equivariant & Invariant

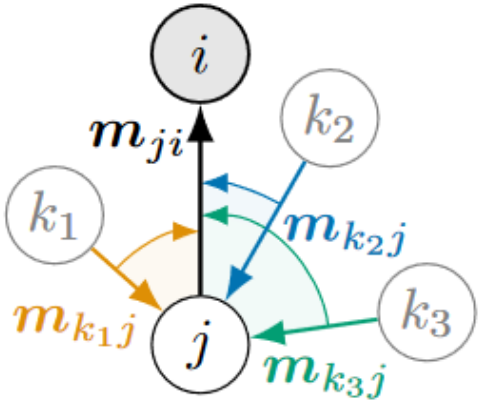
❑Invariant Models

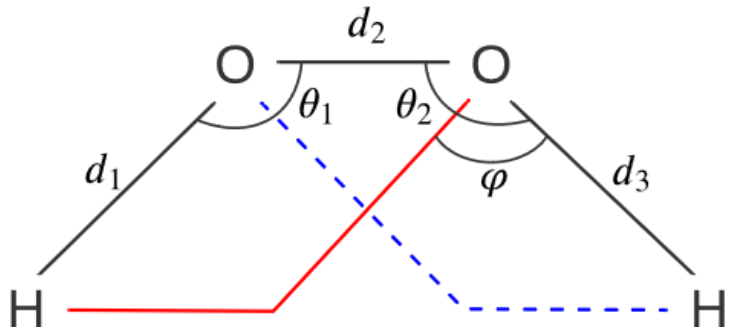
– Extracting geometric information from CCS as model input, but previous works cannot achieve molecular **completeness**.

SchNet: distance



DimeNet: angle





Completeness

The structure is determined by all the **distance**, **angle**, and **torsion** information to achieve completeness.

Background: Equivariant & Invariant

❑Equivariant Models

– Using raw coordinate representation in cartesian coordinate system (CCS) as input, so that **each layer has to be designed to be equivariant** to capture the geometric information.

Background: Equivariant & Invariant

❑Equivariant Models

– Using raw coordinate representation in cartesian coordinate system (CCS) as input, so that **each layer has to be designed to be equivariant** to capture the geometric information.

– To achieve completeness, equivariant models require to aggregate edge-based 2-hop information, resulting in complexity of $\mathbf{O(nk^3)}$, where n is the number of nodes, k is the average number of neighbors.

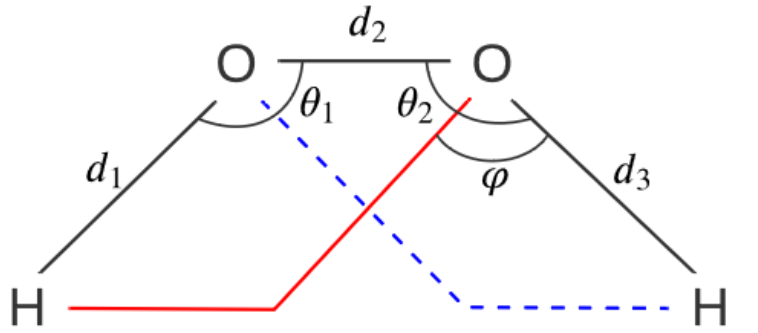
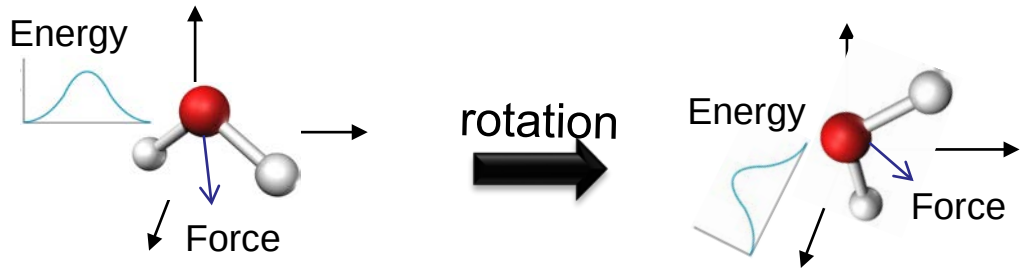


Figure 1: The chemical structure of the H_2O_2.

Background: Equivariant & Invariant

❑Equivariant Models

- Using raw coordinate representation in cartesian coordinate system (CCS) as input, so that **each layer has to be designed to be equivariant** to capture the geometric information.
- To achieve completeness, equivariant models require to aggregate edge-based 2-hop information, resulting in complexity of $\mathbf{O(nk^3)}$, where n is the number of nodes, k is the average number of neighbors.
- Most properties are SE(3) invariant.



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❑ Invariant Models

- Extracting geometric information from CCS as model input, but previous works cannot achieve molecular **completeness**.
- Only need to aggregate 1-hop, but receive 2-hop information.
- Distance (e.g., SchNet, PhysNet), Direction (DimeNet)

Problem Definition

❑ Research Goal

– Propose a 3D message passing scheme that can completely efficiently identify a molecule graph.

❑ Spherical Message Passing

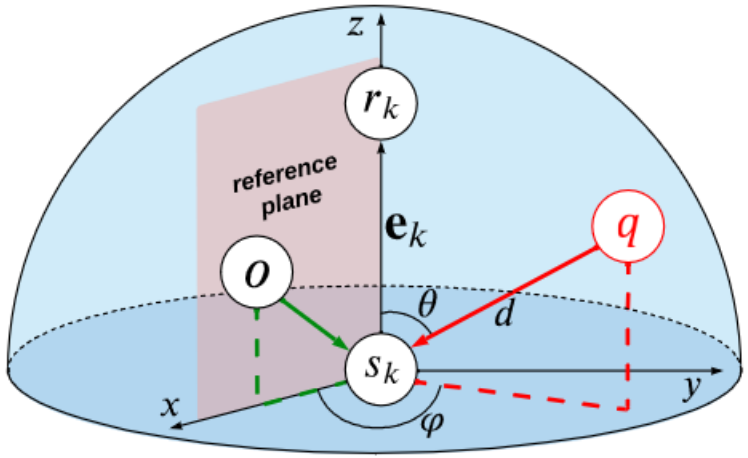
– Consider all the distance, angle, and torsion information

– A novel strategy for computing torsion

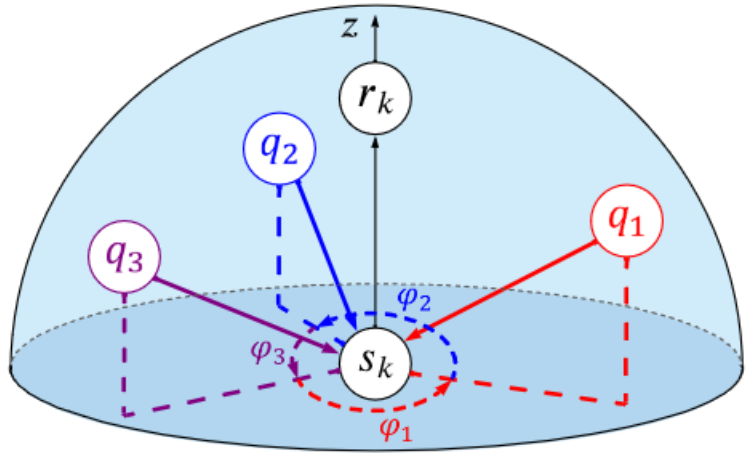
- Approximately complete – can identify chirality
- Efficient – $O(nk^2)$

– Naturally invariant

Invariant model	Completeness
	Efficiency

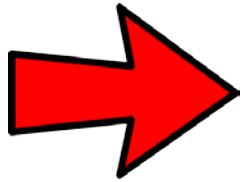


(a)



(b)

Roadmap



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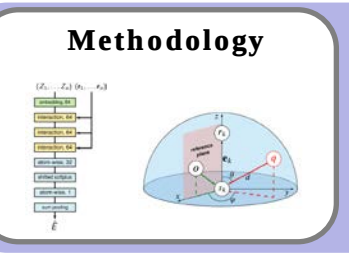

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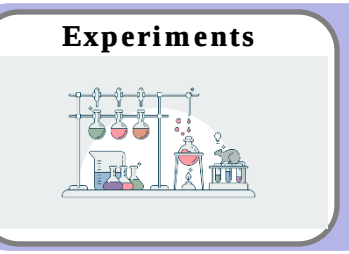

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Complete Representation of Molecules

❑ Invariant representation of molecules in SCS

– Relative information is invariant to transitions and rotations.

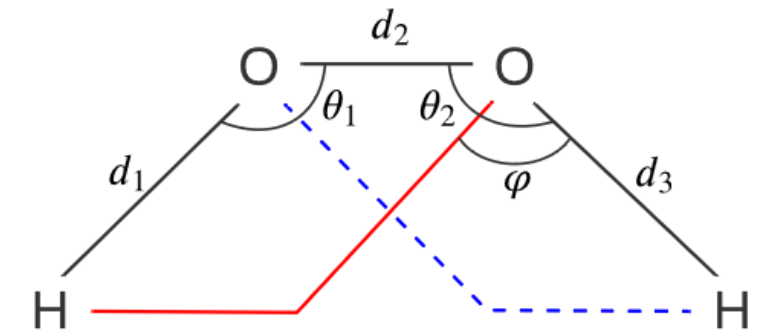

Figure 1: The chemical structure of the H_2O_2.

Atoms in molecule

bond length (d)

bonds angle (θ)

torsion angle (φ)

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- Represent relative information in Spherical coordinate system (SCS)

Points in SCS

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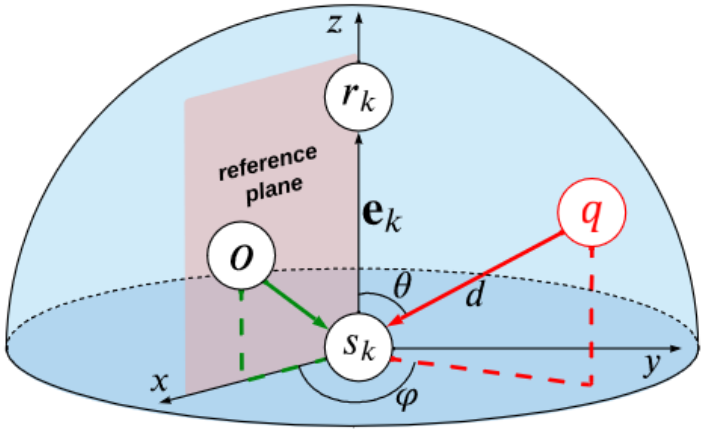

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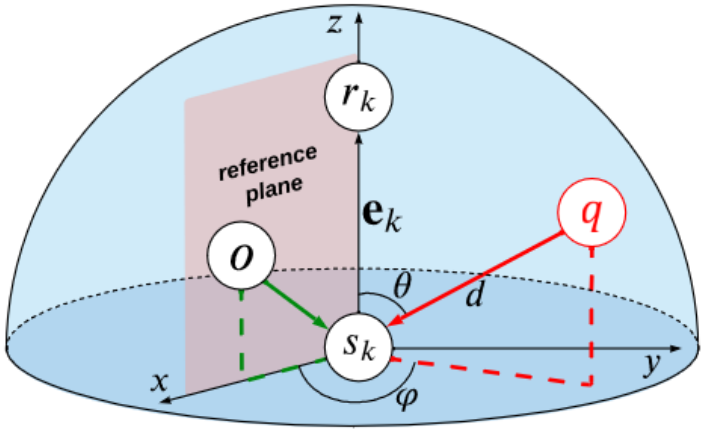

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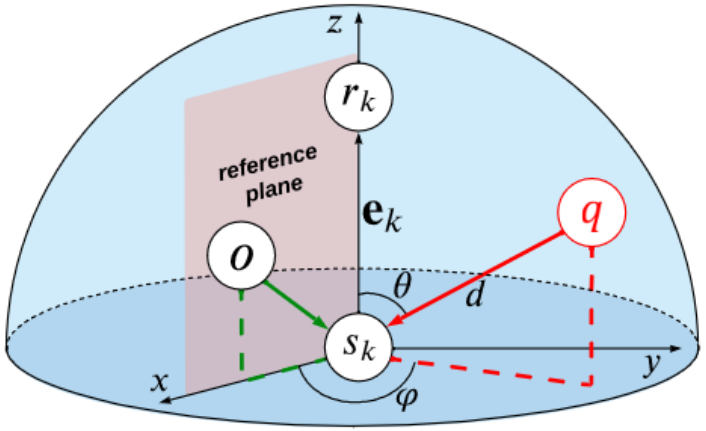

Spherical Message Passing

❑ Notations

- 3D molecule graph: G = (**u**, V, E, P)
- Global graph features: **u**
- Atom features: $V = \{\mathbf{v}_i\}_{i=1:n}$
- Edges: $E = \{(\mathbf{e}_k, r_k, s_k)\}_{k=1:m}$, feature vector:$\mathbf{e}_k$, index: r_k, s_k
- Edge set pointing to *i*-th atom: $E_i = \{(\mathbf{e}_k, r_k, s_k)\}_{r_k=i,k=1:m}$
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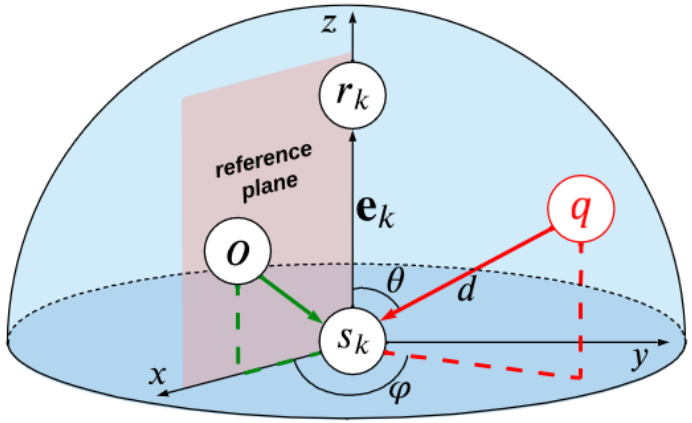

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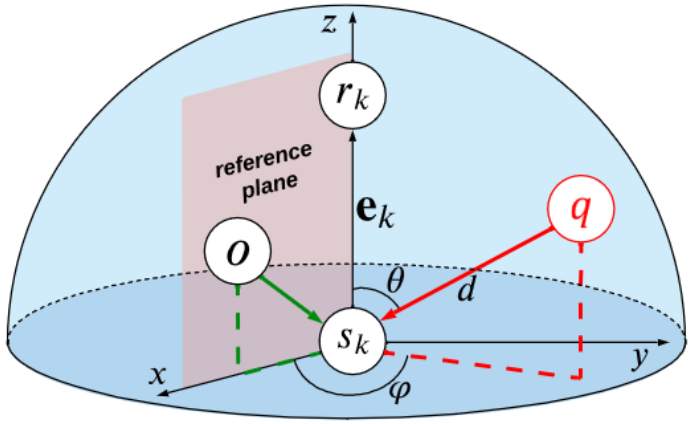
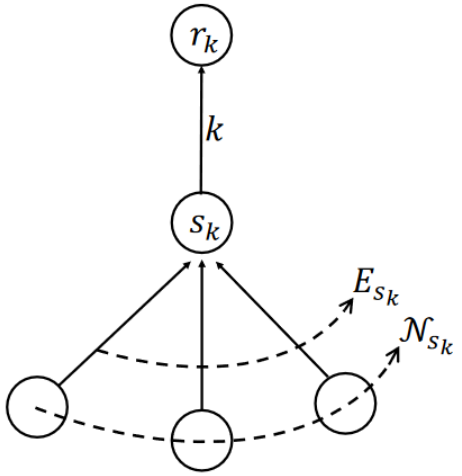


❑ Constructing Spherical coordinate system (SCS)

- Origin: s_k
- Z-axis: e_k
- Reference plane: Reference atom *O*, and r_k, s_k
- Locate any neighbor atom q via 3-tuple (d, θ, φ)



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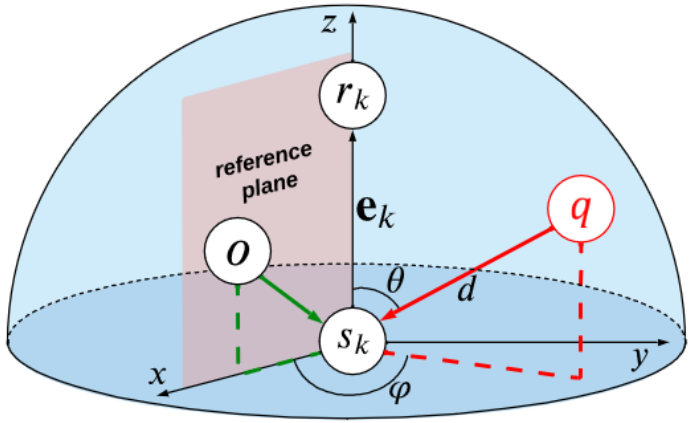
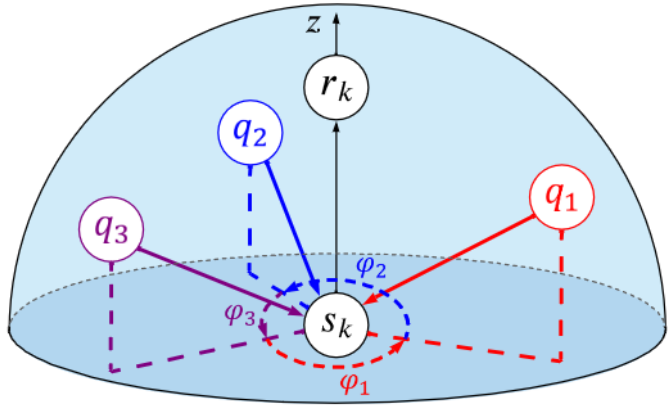


How to define torsion angle for any atom *q*?



Spherical Message Passing

❑ Message Passing Scheme

– Update edges $E = \{(\mathbf{e}_k, r_k, s_k)\}_{k=1:m}$ from position

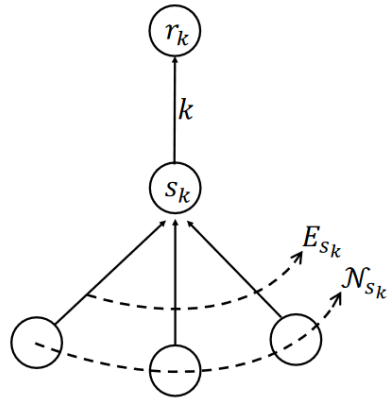
$$\mathbf{e}'_k = \phi^e\left(\mathbf{e}_k, \mathbf{v}_{r_k}, \mathbf{v}_{s_k}, E_{s_k}, \rho^{p\to e}\left(\{\mathbf{r}_h\}_{h=r_k\cup s_k\cup\mathcal{N}_{s_k}}\right)\right),$$

– Update atoms $V = \{\mathbf{v}_i\}_{i=1:n}$ from updated edges.

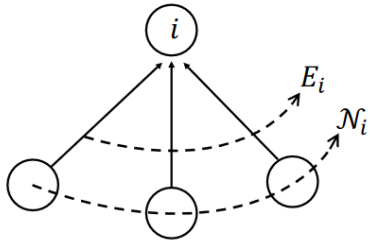
$$\mathbf{v}'_i = \phi^v\left(\mathbf{v}_i, \rho^{e\to v}\left(E'_i\right)\right),$$

– Update molecule feature **u** from atoms

$$\mathbf{u}' = \phi^u\left(\mathbf{u}, \rho^{v\to u}\left(V'\right)\right),$$



(a)



(b)

Spherical Message Passing

❑ Completeness vs. Efficiency

– **Efficiency:**

- Previous complete representation (equivariant GNNs) requires edge-based 2-hop information, so it's time complexity is: $O(nk^3)$. They cannot scale to large molecules.

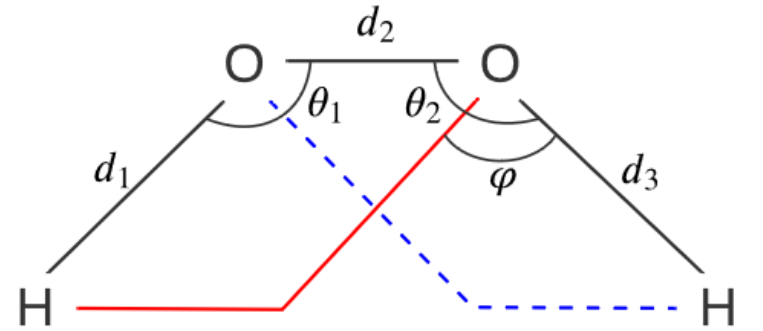


Figure 1: The chemical structure of the H_2O_2.

Spherical Message Passing

❑ Completeness vs. Efficiency

– **Efficiency:**

- Previous complete representation (equivariant GNNs) requires edge-based 2-hop information, so it's time complexity is: $O(nk^3)$. They cannot scale to large molecules.
- SMP only involves edge-based 1-hop information, thus the time complexity is reduced to $O(nk^2)$

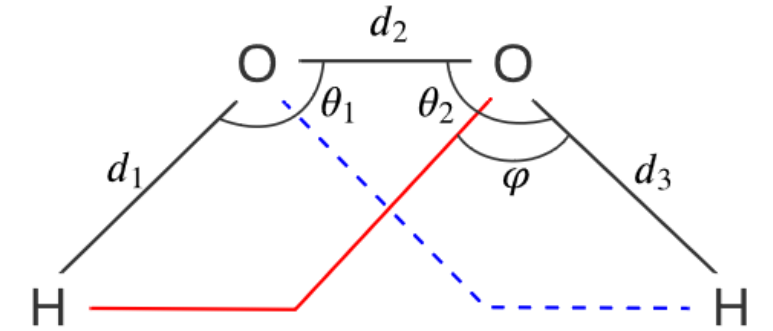
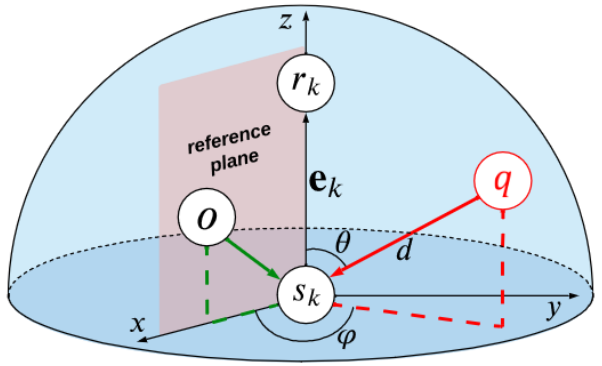


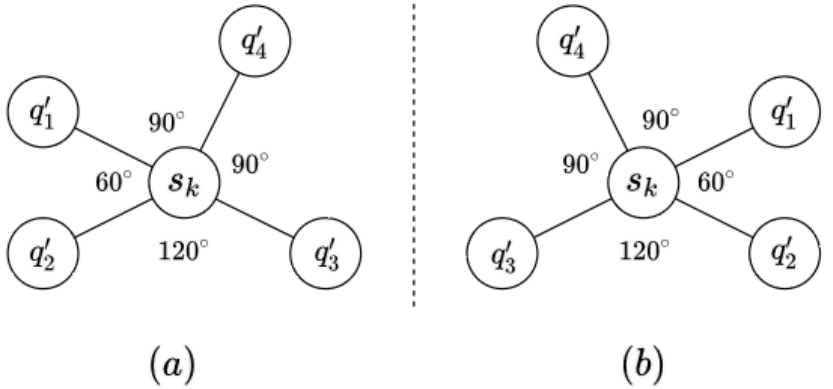
Figure 1: The chemical structure of the H_2O_2.



Spherical Message Passing

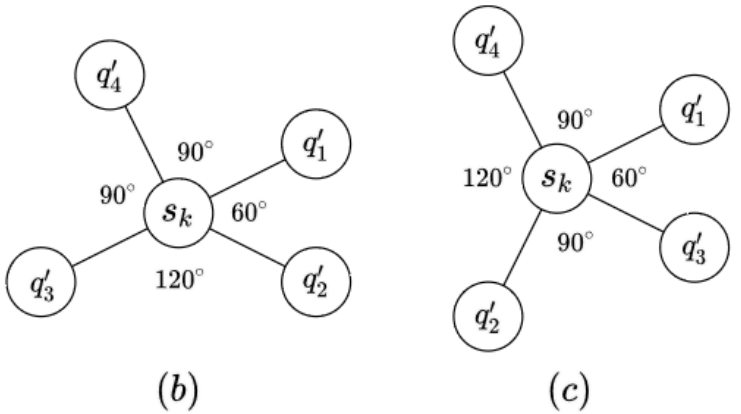
❑ Completeness vs. Efficiency

- **Efficiency:**
  - Previous complete representation: $O(nk^3)$.
  - SMP: $O(nk^2)$.
- **Completeness:**
  - √ SMP can distinguish even complex geometric properties such as **chirality**, (a) and (b).
  - × SMP does not consider absolute orders of torsion angles, (b) and (c), But this may not exit in nature.
  - SMP achieves approximate completeness



(a) $q'_1(90°), q'_2(60°), q'_3(120°), q'_4(90°)$

(b) (c) $q'_1(60°), q'_2(120°), q'_3(90°), q'_4(90°)$



SphereNet

❑ Physically-based representation of (d, θ, φ)

– The obtained 3-tuple (d, θ, φ) indicates the relative location of any atom in a 3D molecular graph. However, it cannot serve as the direct input to neural networks, as it lacks meaningful representations.

How to transform 3-tuple (d, θ, φ) to meaningful representations?

– Molecules are quantum systems thus the representation design needs to follow physics laws.

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Spherical Bessel function Spherical Harmonic function

$$\Psi(d, \theta, \varphi) = j_\ell \left(\frac{\beta_{\ell n}}{c} d \right) Y_\ell^m(\theta, \varphi)$$

David J. Griffiths and Darrell F. Schroeter. Introduction to Quantum Mechanics. 3 edition, August 2018.
Johannes Klicpera, Janek Groß, and Stephan Günnemann. Directional message passing for molecular graphs. ICLR, 2020.

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Spherical Bessel function

Spherical Harmonic function

Torsion angle $\Psi(d, \theta, \varphi) = j_\ell\left(\frac{\beta_{\ell n}}{c} d\right) Y_\ell^m(\theta, \varphi)$

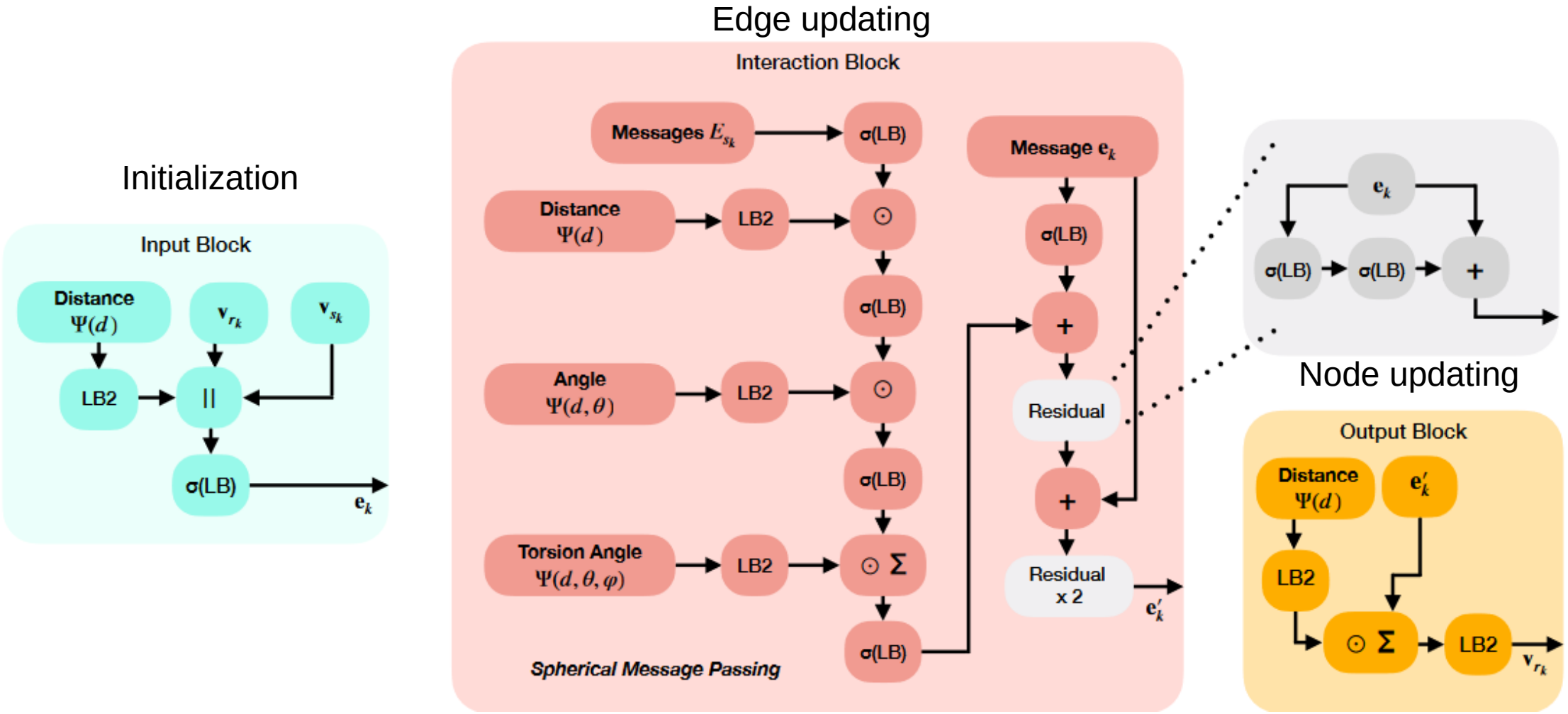
Bond angle $\Psi(d, \theta)$

Bond distance $\Psi(d)$

David J. Griffiths and Darrell F. Schroeter. Introduction to Quantum Mechanics. 3 edition, August 2018.
Johannes Klicpera, Janek Groß, and Stephan Günnemann. Directional message passing for molecular graphs. ICLR, 2020.

SphereNet: Framework

Spherical message passing (approximately complete) + Physically based representation (meaningful)



Relation to SchNet

SchNet can be derived from the proposed Spherical Message Passing scheme.

1. Update edge feature

$$\mathbf{e}'_k = \phi^e\left(\mathbf{e}_k, \mathbf{v}_{r_k}, \mathbf{v}_{s_k}, E_{s_k}, \rho^{p\to e}\left(\{\mathbf{r}_h\}_{h=r_k\cup s_k\cup\mathcal{N}_{s_k}}\right)\right),$$

$$\begin{aligned}\mathbf{e}'_k =& \phi^e\left(\mathbf{v}_{r_k}, \rho^{p\to e}\left(\{\mathbf{r}_h\}_{h=r_k\cup s_k}\right)\right)\\ =& \phi^e\left(\mathbf{v}_{r_k}, \Psi\left(\|\mathbf{r}_{s_k}-\mathbf{r}_{r_k}\|\right)\right)\\ =& \mathrm{NN}\left(\mathrm{NN}\left(\mathbf{v}_{r_k}\right)\odot \mathrm{NN}\left(\Psi\left(\|\mathbf{r}_{r_k}-\mathbf{r}_{s_k}\|\right)\right)\right),\end{aligned}$$

2. Update atom feature

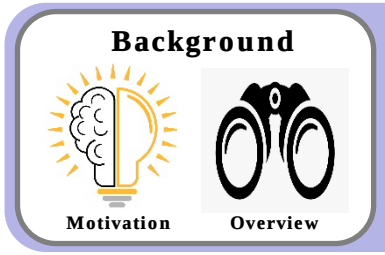
$$\mathbf{v}'_i = \phi^v\left(\mathbf{v}_i, \rho^{e\to v}\left(E'_i\right)\right),$$

$$\begin{aligned}\mathbf{v}'_i =& \phi^v\left(\mathbf{v}_i, \rho^{e\to v}\left(E'_i\right)\right)\\ =& \phi^v\left(\mathbf{v}_i, \sum_{\left(\mathbf{e}'_k, r_k, s_k\right)\in E'_i}\mathbf{e}'_k\right)\\ =& \mathbf{v}_i + \sum_{\left(\mathbf{e}'_k, r_k, s_k\right)\in E'_i}\mathbf{e}'_k,\end{aligned}$$

3. Update graph feature

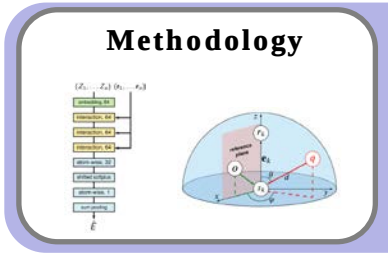
$$\begin{aligned}\mathbf{u}' =& \phi^u\left(\mathbf{u}, \rho^{v\to u}\left(V'\right)\right),\\ \mathbf{u} =& \phi^u\left(\rho^{v\to u}\left(V^T\right)\right)\\ =& \sum_{i=1:n}\mathrm{NN}\left(\mathbf{v}_i^T\right).\end{aligned}$$

Roadmap



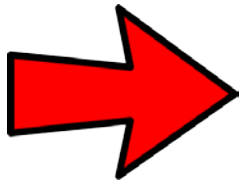
I. Background

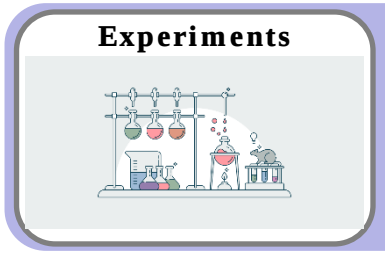
- Message Passing Scheme
- 3D Graph



II. Spherical Message Passing for 3D Molecular Graphs

- Background & Motivation
- Spherical Message Passing Scheme & Completeness
- SphereNet





III. Experiments & Analysis

- Datasets & Tasks
- Completeness vs. Efficiency
- Ablation Study

IV. Conclusion

Experiments: Comparison on three Tasks:

- **OC20**: Tasks: S2EF, **IS2RS**, and IS2RE. IS2RS predicts structure's energy in the relaxed state.
  - Training set: 4630,318 sctructures
  - Evaluation set: In Domain (ID), Out of Domain Adsorbates (OOD Ads), Out of Domain catalysts (OOD cat), and Out of Domain Adsorbates and catalysts (OOD Both), where numbers of structures are 24,943, 24,961, 24,963, 24,987, respectively.
  - Energy MAE and the percentage of Energies within a Threshold (EwT) of the ground truth energy
- **QM9**: Task: Property prediction. Consists organic molecules composed of up to 9 heavy atoms
  - Training set: 110,000
  - Validation and Test set: 10,000 & 10831 structures.
- **MD17**: Task: Molecular dynamic simulation.
  - Training: 1000 for training.

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Energy MAE: the best performance on 3 out of 4 splits, reduces the average energy MAE by 0.019, which is 3.10% of the second best model.
EwT: the best on all the 4 splits. it improves the average EwT from 3.42% to 3.64%, which is a large margin considering the inherently low EwT values.

	Energy MAE [eV] ↓					EwT ↑				
Model	ID	OOD Ads	OOD Cat	OOD Both	Average	ID	OOD Ads	OOD Cat	OOD Both	Average
CGCNN	0.6203	0.7426	0.6001	0.6708	0.6585	3.36%	2.11%	3.53%	2.29%	2.82%
SchNet	0.6465	0.7074	0.6475	0.6626	0.6660	2.96%	2.22%	3.03%	2.38%	2.65%
DimeNet++	0.5636	0.7127	0.5612	0.6492	0.6217	4.25%	2.48%	4.40%	2.56%	3.42%
GemNet-T	**0.5561**	0.7342	0.5659	0.6964	0.6382	4.51%	2.24%	4.37%	2.38%	3.38%
SphereNet	0.5632	**0.6682**	**0.5590**	**0.6190**	**0.6024**	**4.56%**	**2.70%**	**4.59%**	**2.70%**	**3.64%**

Experiments: Comparison on three Tasks:

- **QM9**: Task: Property prediction. Consists organic molecules composed of up to 9 heavy atoms
  - Training set: 110,000
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Property	Unit	PPGN	SchNet	PhysNet	Cormorant	MGCN	DimeNet	DimeNet++	PaiNN	**SphereNet**
μ	D	0.047	0.033	0.0529	0.13	0.0560	0.0286	0.0297	**0.012**	0.0245
α	$a_0{}^3$	0.131	0.235	0.0615	0.092	**0.0300**	0.0469	0.0435	0.045	0.0449
ϵ_{HOMO}	meV	40.3	41	32.9	36	42.1	27.8	24.6	27.6	**22.8**
ϵ_{LUMO}	meV	32.7	34	24.7	36	57.4	19.7	19.5	20.4	**18.9**
$\Delta\epsilon$	meV	60.0	63	42.5	60	64.2	34.8	32.6	45.7	**31.1**
$\langle R^2 \rangle$	$a_0{}^2$	0.592	0.073	0.765	0.673	0.110	0.331	0.331	**0.066**	0.268
ZPVE	meV	3.12	1.7	1.39	1.98	**1.12**	1.29	1.21	1.28	**1.12**
U_0	meV	36.8	14	8.15	28	12.9	8.02	6.32	**5.85**	6.26
U	meV	36.8	19	8.34	-	14.4	7.89	6.28	**5.83**	6.36
H	meV	36.3	14	8.42	-	14.6	8.11	6.53	**5.98**	6.33
G	meV	36.4	14	9.40	-	16.2	8.98	7.56	**7.35**	7.78
c_{v}	$\frac{\text{cal}}{\text{mol K}}$	0.055	0.033	0.0280	0.031	0.0380	0.0249	0.0230	0.024	**0.0215**
std. MAE	%	1.84	1.76	1.37	2.14	1.86	1.05	0.98	1.01	**0.91**

SphereNets achieves best performance on 5 properties and the second best performance on 3 properties.

Experiments: Comparison on three Tasks:

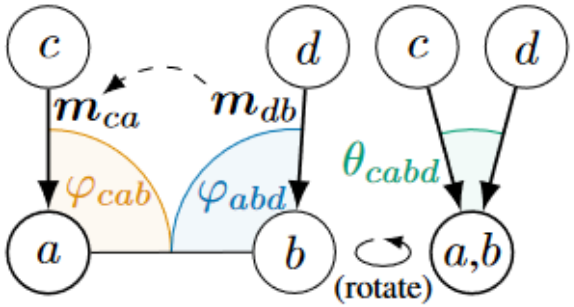
- **MD17**: Task: Molecular dynamic simulation.
  - Training: 1000 for training. WoFE: weight of force
  - sGDML is one of the original work that created the MD17 dataset with carefully-designed features.

	WoFE = 100				WoFE = 1000			
Molecule	sGDML	SchNet	DimeNet	**SphereNet**	NequIP	GemNet-T	GemNet-Q	SphereNet
Aspirin	0.68	1.35	0.499	**0.430**	0.353	0.220	0.217	0.209
Benzene	0.20	0.31	0.187	**0.178**	0.186	0.145	0.145	0.147
Ethanol	0.33	0.39	0.230	**0.208**	0.204	0.086	0.088	0.091
Malonaldehyde	0.41	0.66	0.383	**0.340**	0.328	0.155	0.160	0.172
Naphthalene	**0.11**	0.58	0.215	0.178	0.105	0.055	0.051	0.048
Salicylic acid	**0.28**	0.85	0.374	0.360	0.242	0.127	0.125	0.113
Toluene	**0.14**	0.57	0.216	0.155	0.102	0.060	0.060	0.054
Uracil	**0.24**	0.56	0.301	0.267	0.173	0.097	0.104	0.106
std. MAE	1.11	2.38	1.10	**0.97**	0.79	0.45	0.45	0.44

WoFE = 100: SphereNet achieves best except comparing to sGDML.
WoFE = 1000: SphereNet achieves similar results with GemNet in spite of that GemNet-T is of high complexity and contains carefully designed network components for performance boost.

Experiments: Completeness vs. Efficiency

Q-MP: Q-MP in GemNet represents the edge-based 2-hop geometric message passing and can generate **complete representations** of 3D molecular graphs.



SMP performs similarly with Q-MP even though the latter is complete theoretically but not scalable in practice.

Table 4: Comparisons bewtween SMP and Q-MP on MD17 using two backbone networks.

	SphereNet Backbone		GemNet Backbone	
Molecule	SMP	Q-MP	SMP	Q-MP
Aspirin	0.209	0.247	0.225	0.231
Benzene	0.147	0.153	0.144	0.149
Ethanol	0.091	0.102	0.089	0.083
Malonaldehyde	0.172	0.168	0.169	0.176
Naphthalene	0.048	0.057	0.063	0.062
Salicylic acid	0.113	0.125	0.111	0.114
Toluene	0.054	0.043	0.052	0.063
Uracil	0.106	0.106	0.098	0.113
Time/Epoch (s)	324	1270	295	1185

Johannes Klicpera, Florian Becker, and Stephan Günnemann. Gemnet: Universal directional graph neural networks for molecules. arXiv preprint arXiv:2106.08903, 2021.

Experiments: Completeness vs. Efficiency

SphereNet uses similar computational resources as DimeNet++ and GemNet-T, and is much more efficient than DimeNet. The main reason could be sphereNet developed an efficient way to compute torsion

Table 9: Efficiency comparisons between SphereNet and other models in terms of number of parameters and time cost per epoch using the same infrastructure.

	SchNet	DimeNet	DimeNet++	GemNet-T	SphereNet
#Param.	185,153	2100,070	1887,110	2040,194	1898,566
Time (s)	100	840	240	290	340

Johannes Klicpera, Florian Becker, and Stephan Günnemann. Gemnet: Universal directional graph neural networks for molecules. arXiv preprint arXiv:2106.08903, 2021.

Experiments: Completeness vs. Efficiency

❑ Ablation Study

– MD17: Task: Molecular dynamic simulation.

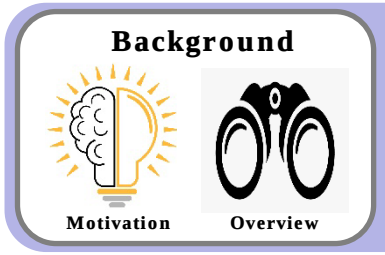
- Training: 1000 for training.
- MAE of forces.

Table 5: Comparisons among three message passing strategies on the same SphereNet architecture on the partial MD17 dataset.

Molecule	SMP w/o (θ, φ)	SMP w/o φ	SMP
Ethanol	0.249	0.22	0.208
Malonaldehyde	0.550	0.360	0.340
Naphthalene	0.372	0.205	0.178
Toluene	0.446	0.182	0.155

These results demonstrate the effectiveness of angle and torsion information used in the SMP. The best performance of SMP further reveals that SMP represents an accurate scheme for 3D graphs.

Roadmap



I. Background

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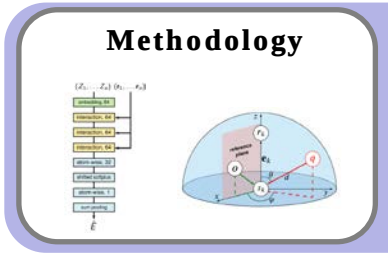
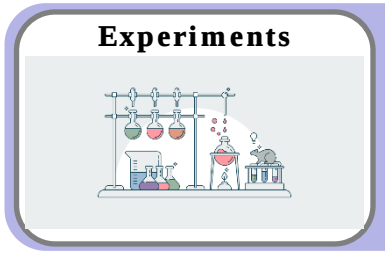
- 3D Graph



II. Spherical Message Passing for 3D Molecular Graphs

- Background & Motivation
- Spherical Message Passing Scheme & Completeness
- SphereNet



III. Experiments & Analysis

- Ablation Study
- Completeness VS Efficiency

IV. Conclusion

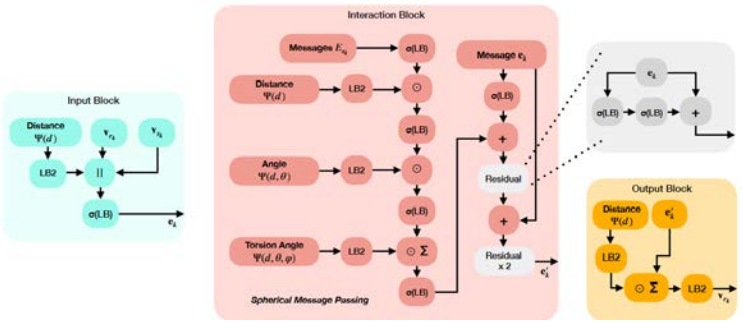
Conclusion

❑ Solved Problems

- How to represent a 3D molecule in Spherical coordinate system?
- How to integrate completeness and efficiency into one SE(3) invariant GNN?

❑ Framework: SphereNet

- Proposed a 3D molecule message passing scheme, Spherical Message Passing, which achieves $O(nk^2)$ efficiency and approximate completeness.
- Further proposed SphereNet based on the SMP (approximately complete) and physical-based representation (meaningful).
- Theoretically analyzed the relation with prior works (SchNet)



❑ Experiments

- Achieves best or second performance on 3 datasets and tasks.
- Efficiency & Scalability: SMP achieves similar performance with Q-MP on MD17, even though the latter is complete theoretically but not scalable in practice.

Thanks!

Jianpeng Chen

CS, Virginia Tech

02/14/2024