Type	Method	Atom Stable (%) ↑	Mol Stable (%) ↑
Normalizing flow	E-NF	75.0	0
DDPM	EDM	81.3	0.0
	Bridge+Force	82.4±0.8	0.0
	GCDM	86.4±0.2	3.7±0.3
	GeoLDM	84.4	3.2
Ours	GFMDiff	**86.5**±0.2	**3.9**±0.2
Data		86.5	2.8

Table 3: Performance comparison on GEOM-Drugs. Results of 10000 generated samples are reported with standard deviations across 3 runs using different seeds.

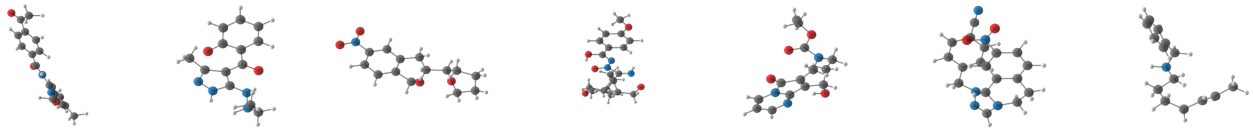

Figure 6: Molecule samples generated by GFMDiff for GEOM-Drugs

Conditional Molecule Generation on GEOM-QM9

For conditional molecule generation on QM9, we compare our GFMDiff with existing methods along with naive baselines. In Table **??**, we show the comparison of MAE on property prediction task. The "Naive (Upper-bound)" is a baseline where samples and labels are shuffled and the "#Atoms" is the property prdiction method which simply relies of the number of atoms. Lower mean absolute errors of a model than these two baselines indicate the model is capable to incorporate properties and molecule conformation information into generated samples.

As it is demonstrated in Table **??**, our methods outperforms the state-of-the-art method in this task. Samples of samples with various values of α is shown in Figure **??** as well. The performence lead of GFMDiff over the second-best method on for 6 properies are 11.7%, 4.9%, 6.2%, 10.2%, 13.7%, and 13.9%, respectively. Results indicates the superiority of our GFMDiff in generate molecules with desirable properties.

De Novo Molecule Generation on GEOM-Drugs

It is a challenging task to generate molecules for GEOM-Drugs dataset, since it is a large scale dataset of big molecules with up to 181 atoms. The relatively large scale of molecules and low stabilities of ground truth data bring huge challenges to 3D molecule generation. In experiments on GEOM-Drugs, we compares GFMDiff with E-NF, EDM, Bridge + Force, GCDM, and GeoLDM. Since current methods performs poorly in the novelty of molecules, we only list the stability of generated samples for comparison.

Due to the size of molecules in GEOM-Drugs, the stability of ground truth data are much lower than that in QM9. The proposed GFMDiff outperforms GCDM in terms of atom stability by a small margin, while GFMDiff outperforms the second-best result on molecule stability by 5.4%. It's worth noting that GeoLDM, which generates samples with high stabilities on QM9, encounters a bottleneck in generating large molecules. Some samples generated by GFMDiff are shown in Figure **??**. Results on Drugs also demonstrate the capability of our proposed GFMDiff to generate stable molecule geometries.

Conclusion

In this paper, we propose GFMDiff, a novel molecule generation methods that fully excevates geometric information to help expressive representation learning and accurate bonds formation in molecule graphs. Unlike earlier methods that did not comprehensively model molecular geometries and heavily rely on predefined rules to generate bonds, GFMDiff makes full use of spatial information to assist on representation learning and facilitate accurate edge generation. We adopt DTN as the denoising kernel to update atom features and coordinates based on interatomic forces and multi-body interactions. The GFLoss is also implemented to actively intervene the formation of bonds during each time step at the training stage. We conduct comprehensive experiments to evaluate the effectiveness and performance edge of the proposed techniques over SOTA methods. It is shown that GFMDiff is capable to generate valid molecules with accurate conformations and correct atom valencies.

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