

Geometric Latent Diffusion Models for 3D Molecule Generation

1. Potential application of the framework of Latent variable + DM to other fields:
 - What are the key aspects need to be considered, e.g. KL-reg vs ES-reg
2. The correlation between latent space learning and the final model performance
 - keeping the encoder untrained (only train the decoder) leads to similar results
3. In the Controllable Molecule Generation task on QM9, there is large discrepancy between the properties of molecules generated by the model and the standard values.
 - Is it acceptable or useful for chemists?