# Non-Autoregressive Electron Redistribution Modeling for Reaction Prediction

Hangrui Bi*, Hengyi Wang*, Chence Shi,
Connor Coley, Jian Tang, Hongyu Guo


北京大学
PEKING UNIVERSITY

Mila

Université de Montréal

Massachusetts Institute of Technology

CIFAR

HEC MONTRÉAL

Canada
NRC·CNRC

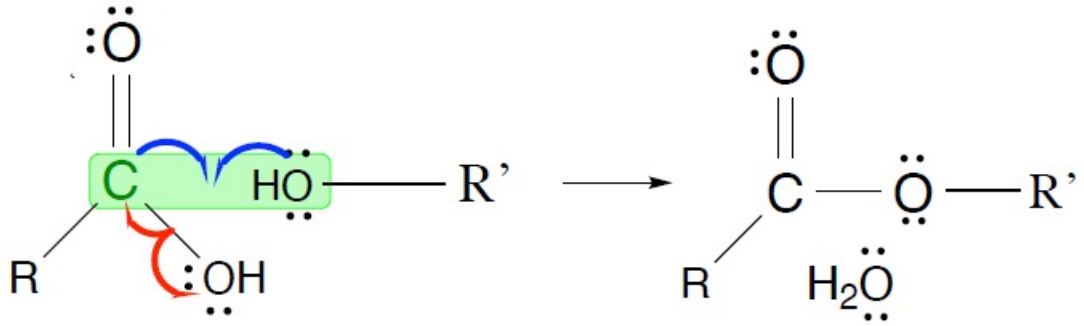
# Motivation

- Predicting the products of chemical reactions presents a fundamental challenge in computational chemistry.
- Existing machine learning approaches typically produce a reaction product by sequentially forming its subparts or intermediate molecules.
- Such autoregressive methods not only require an arbitrary order for the incremental construction but also preclude the use of parallel decoding for efficient computation.
- To address these issues, we devise a transformer-like network to generate low-degree molecule graphs non-autoregressively

# Methods

- Chemical bonds are typically pairs of shared electrons. Bonds formed/broken can be expressed as reaction electron flows.

- We employ a multi-pointer network, whose multiple attention heads indicate the direction of electron flows



# Results

| Model Name(scheme) | Accuracies(%) | | | | parallel | end-to-end |
|---|---|---|---|---|---|---|
| | Top-1 | Top-2 | Top-3 | Top-5 | | |
| WLDN† (combinatorial) | 79.6 | - | 87.7 | 89.2 | ✓ | × |
| GTPN †( graph) | 83.2 | - | 86.0 | 86.5 | × | ✓ |
| Transformer-base † ( sequence) | 88.8 | 92.6 | 93.7 | 94.4 | × | ✓ |
| MEGAN†(graph) | 89.3 | 92.7 | 94.4 | **95.6** | × | ✓ |
| Transformer-augmented †( sequence) | 90.4 | **93.7** | **94.6** | 95.3 | × | ✓ |
| Symbolic† (combinatorial) | 90.4 | 93.2 | 94.1 | 95.0 | ✓ | × |
| NERF | **90.7**±0.03 | 92.3±0.22 | 93.3±0.15 | 93.7±0.17 | ✓ | ✓ |

| Model Name | Wall-time | Latency | Speedup |
|---|---|---|---|
| Transformer (b=5) | 9min | 448ms | 1 × |
| MEGAN (b=10) | 31.5min | 144ms | 0.29 × |
| Symbolic | >7h | 1130ms | 0.02 × |
| NERF | 20s | 17ms | 27× |

† indicates that the results were copied from its published paper.