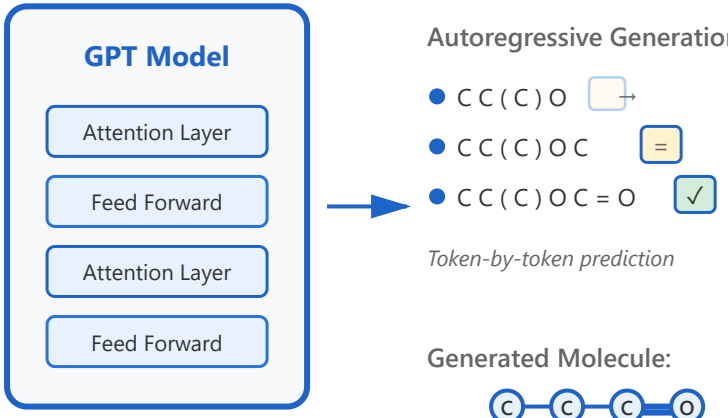
GPT for Molecules

SMILES Generation Process



Chemical language models

ChemGPT, MolGPT architectures

Property conditioning

Control molecular attributes

Reaction prediction

Reactants → Products mapping

Retrosynthesis

Backward synthesis planning