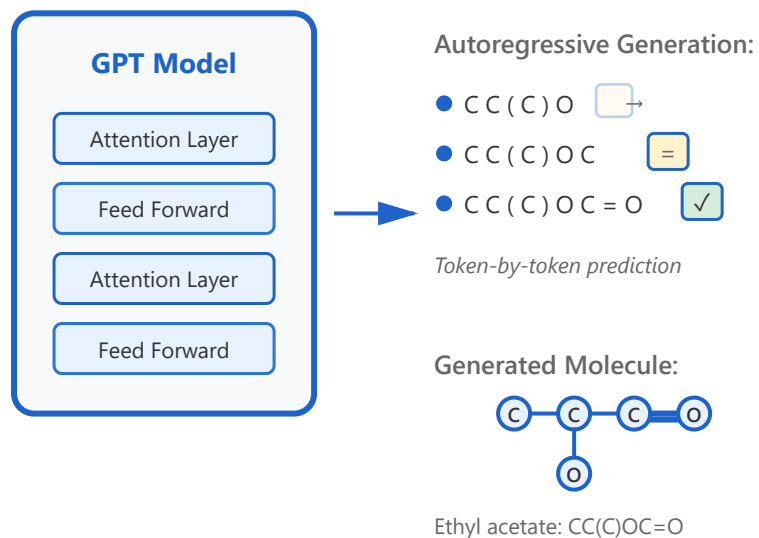


# GPT for Molecules

## SMILES Generation Process



### Chemical language models

ChemGPT, MolGPT architectures

### Property conditioning

Control molecular attributes

### Reaction prediction

Reactants → Products mapping

### Retrosynthesis

Backward synthesis planning