Transformer-based Polymer Property Prediction System Architecture

User Roles

- Scientists
- Engineers
- Researchers
- Admin

Frontend
React.js

- SMILES Input
- Results Display
- History View

Backend
Node.js + Express

- API Gateway
- Auth Service
- DB Controller

ML API
Flask/FastAPI

- API Endpoints
- SMILES Validator
- Model Interface

ML Model Pipeline

SMILES Tokenizer → Transformer Model → Property Predictor → Evaluation → Model Storage

Database Layer

- MongoDB
- User Queries
- Data Storage