AI-based Automated Screening Pipeline

Industrial Waste Database (16 candidates) → **Structure Generation (Pymatgen)** → **CHGNet Optimization (GPU-accelerated)**

Hydration System Creation (+10 H_2O) → **MD Simulation (NVT, 10 ps) CHGNet MLP** → **Multi-metric Analysis (Ca, Si, C-S-H)**

Scoring & Ranking (A/B/C grades)