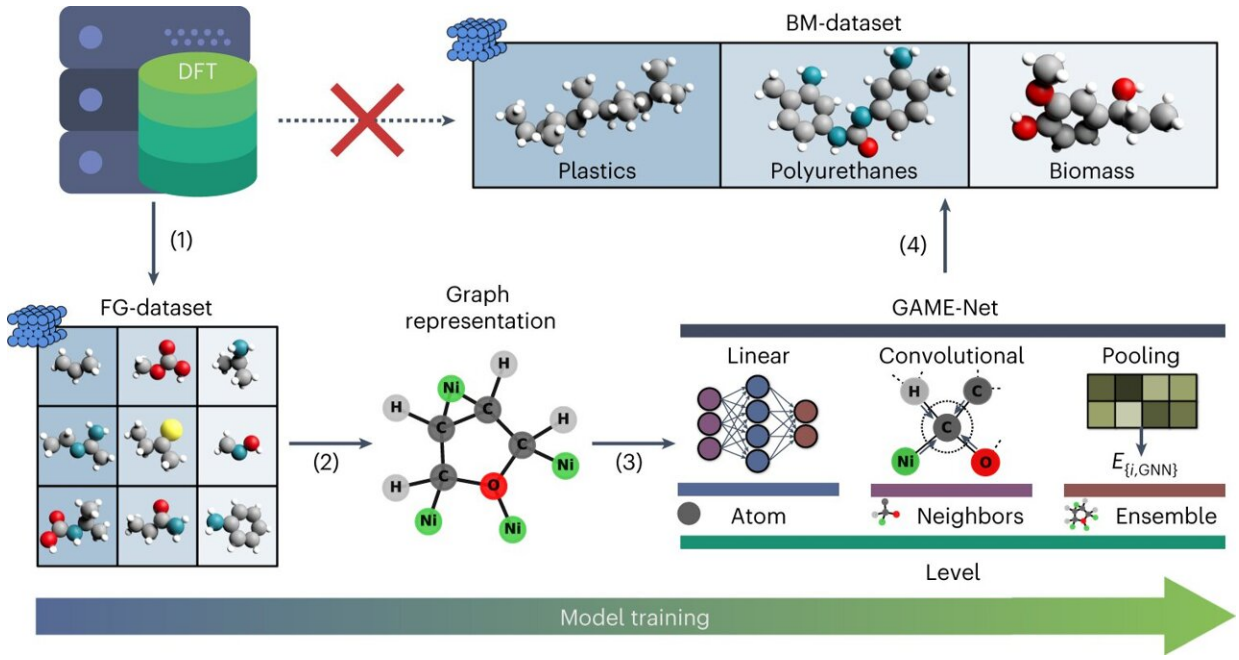
A graph neural network for fast evaluation of the adsorption energy in heterogeneous catalysis

May 2 2023, by Laura Hernández Eguía



Schematic illustration of the workflow for GAME-Net. Starting from the DFT FG-dataset containing small adsorbates (3,315 points; step 1), we transform the sample adsorption systems to their corresponding graph representation (molecule and metal atoms directly interacting with the adsorbate) (step 2) to train the proposed GNN architecture (step 3). The final purpose is using GAME-Net to estimate the adsorption energy of big molecules C

network-fast-adsorption.html