# Computational study of catalytic urethane synthesis

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Polyurethanes (PU) are versatile materials utilized in construction, automotive, and medical industries, are synthesized from polyols and diisocyanates with the aid of catalysts and other additives. Despite their widespread use, understanding the molecular mechanisms underlying polyurethane synthesis is critical to advancing their properties and sustainability. To address this, we conducted a computational investigation into the general mechanism of catalytic urethane formation. Using theoretical methods, we examined the reaction between model compounds such as phenyl isocyanate and butan-1-ol, both in the absence of catalysts and in the presence of various catalysts. Thermodynamic properties of the reactions were calculated using the G3MP2BHandHLYP composite method. Among the catalysts studied, acid and amine catalysts were particularly interesting due to their applicability in industrial polyurethane synthesis. This study provides insights into the molecular-level synthesis of polyurethanes, contributing to the development of more efficient and environmentally friendly materials.