Catalysis/Materials Science Meets Artificial Intelligence:
A New Path for Sustainability

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Catalysis is a sub-discipline of materials science. Catalysis contributes ~35% of World GDP or $ 27 Trillion/yr. Nearly 95% of products, 70% processes use catalysis. Climate Change, Environmental Protection and Sustainable Energy and Chemicals are critical concerns that can effectively be addressed by catalysis. However, in spite of 100 years of research and 10+ Nobel Prizes, catalyst discovery and development remains an empirical science. Catalysts generally takes decades from discovery to commercialization. Today, with the infusion of Artificial Intelligence (AI)/Machine Learning (ML) into High-Throughput (HT) methods and Robotics promises to create a renaissance in catalysis research and development. Following a brief discussion of each of these areas, examples of applications to catalysis will be presented.