Evolution of Computational Chemistry:
UNDERSTANDING CONCEPT TO EXPEDITING COMMERCIALIZATION

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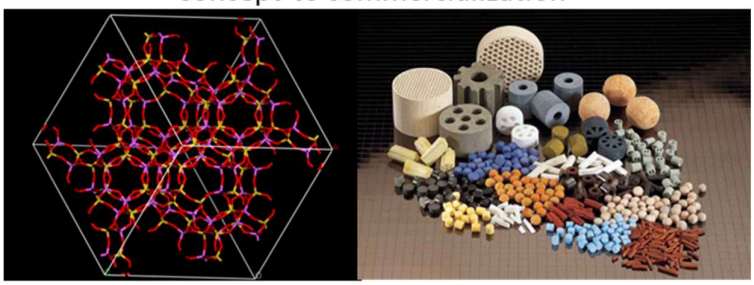
This talk is about the application of computational chemistry for developing **two commercial catalysts**. **First,** a silver catalyst for epoxidation of ethylene' where the product ethylene oxide is the monomer for making PET - the world's fastest-growing packaging plastic. Silver and only silver is used as the main ingredient of the catalyst to make ~31 million metric tonnes of EO per year at the rate of 1,300 USD per metric tonne. [Ref. https://www.statista.com/statistics/1245260/ethylene-oxide-market-volume-worldwide/ ; https://www.chemanalyst.com/Pricing-data/ethylene-oxide-1102]

Second, a cobalt catalyst for the hydrogenation of carbon monoxide which leads to the formation of high-quality gasoline. Cobalt is used as the main ingredient of the catalyst to make 140,000 barrels per day (8.125 billion litres per year) of artificial petroleum liquid in the world's second-largest plant in Qatar. [Ref. https://en.wikipedia.org/wiki/Fischer%E2%80%93Tropsch_process#:~:text=It%20uses%20cobalt%20catalysts%20at,natural%20gas%20liquids%20and%20ethane.]

Concept to commercialization



Ref.:
R. Vetrivel, Studies in Surface Science and Catalysis, 113 (1998) 127-138

Ref.:
https://www.oilandgasmiddleeast.com/news/article-9496-top-10-catalysts-companies

Computational chemistry benefited from the growth of computing power. It is evident from the growth from IBM370 in the 1970s to today's high-performance computers (HPC) @ IITM. Integrating computational chemistry with experimental approaches is the key to success, which was also taught by Professor B. Viswanathan.

Biography of the Speaker: Dr. Rajappan Vetrivel, an Honorary Professor at Poorna Prajna Institute of Science and Technology, Bangalore, is a distinguished Computational Chemist. Trained at IIT-Madras under Prof. B. Viswanathan, he pioneered molecular modeling departments at institutions like the National Chemical Laboratory, Pune, GE Technology Centre, Bangalore, and Shell Technology Centre, Bangalore. A postdoc with Prof. Richard Catlow, FRS, in the UK, he co-founded Sravathi AI, blending AI with pharmaceuticals and chemicals. Awards include the Catalysis Society of India's 1997 Young Scientist Award, GE and Shell Corporate Share options, and patents. Dr. Vetrivel has authored 125 scientific journal publications and holds 10 patents.