**Ethylene Dimerization: DFT Mechanistic Study and Development of Anti-Fouling Compounds**

**Sibo Lin1, Motaz Khawaji2, Mohamed Elanany2, Wei Xu2**

1Aramco Services Company: Aramco Research Center – Boston, Catalysis Technology Group, Cambridge, MA, USA, sibo.lin@aramcoamericas.com

2 Saudi Aramco: Aramco Research Center – KAUST, Chemicals R&D Lab, Thuwal, Saudi Arabia

**Sibo Lin**

**Abstract:** Titanium- and aluminum-catalyzed ethylene dimerization to 1-butene (AlphaButol process) has been practiced industrially for decades, yet inevitable reactor fouling with polyethylene byproduct remains a fundamental challenge. Spectroscopic data has shown that a complex mixture of Ti(III) and Ti(IV) species are formed, depending on the Al/Ti ratio and presence of ligands such as tetrahydrofuran. This concomitant mixture of species has frustrated mechanistic analysis and rational prevention of reactor fouling. Herein, we utilize computational molecular modelling (extended tight binding theory and density functional theory as implemented in XTBDFT) to examine the mechanism of 1-butene and polyethylene formation with computational molecular modelling. From the mechanism, we develop novel anti-fouling compounds that effectively reduce polyethylene formation while retaining or even enhancing 1-butene productivity. This technology has been patented and licensed for industrial implementation.