Computational Materials and Catalysis for Industrial Applications

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This course aims to explore the applications of materials science, catalysis, and chemistry within the energy industry

Following topics will be covered in this course

- Overview of the materials and catalysis in oil and gas /petrochemical industry.
- Role of computational materials, chemistry and catalysis in the industry. Development of Car-Parrinello molecular dynamics and machine learning potentials for materials. Sabatier Principle for optimizing catalysis and material efficiency. Mechanistic (kinetics and thermodynamics) understanding of reaction pathways.
- Introduction to AI/ML for chemistry and materials. Processing-structure-property-performance (PSPP) models for correlating atomic properties to industrial scale. Forward and Inverse ML models for screening/designing molecules and materials.
- Discovery to scaling of molecules and materials. Introduction of technology readiness levels (TRL) of materials.
- The course will focus on certain examples from atomistic scale to commercialization path. How you choose a problem statement in the industry? What kind of technologies are needed? Challenges and mitigation at each TRL stage.
- Group discussions and oral presentations on industrial case studies.
- Industrial Applications: Fischer-Trosch synthesis, CO2 capture and conversion, Haber-Bosch process, Ziegler-Natta, single site catalysts, ethylene oxidation, hydroprocessing (oil to chemicals) and energy storage materials.

References:

1. James A. Kent, Tilak V. Bommaraju, Scott D. Barnicki (Editors). Handbook of Industrial Chemistry and Biotechnology (13th Edition)
   Page 1 – 185, 1695 – 1729, 1781 – 1802.

2. Agrawal et al. APL Mater. **4**, 053208 (2016); https://doi.org/10.1063/1.4946894
3. Fischer-Tropsch : Sayes et al. Chem.Rev.2023,123,5798−5858
4. Redox Flow Battery : Wang. Angew. Chem. 2025, e202515639
5. Ml Potentials : Xia et al Chem. Soc. Rev., 2025, 54, 479
6. Reuter et al. Nature Reviews **| MATERIALS** volume 7 | December 2022 | 991