

Molecular Modeling Improving Vehicle Diagnostic System Sensors

Outcome: Scientists at Louisiana Tech University have used computer modeling to understand the molecular interactions controlling vehicle emissions sensors.

Impact/benefit: Nitrogen oxide (NO_x) exhaust sensors play a critical role in monitoring diesel emissions and communicating with the vehicle diagnostic system to regulate engine operation. Molecular-level understanding of the mechanisms governing the sensors will contribute to the design of sensors with greater sensitivity and accuracy, further reduce air pollution and satisfy future emission requirements.

Explanation: Yttria-stabilized ZrO₂ (YSZ) is commonly used as the sensor electrolyte given its tolerance for the harsh exhaust gas environment. The different modes of operation and variation in microstructures have made it difficult to fully elucidate the role of porous YSZ on gas sensing experimentally. Recent research indicates the microstructure of YSZ plays a role in NO_x sensing, with porosity impeding the ability of certain reactions to proceed, possibly as a result of limited oxygen ion transport.

The computer modeling study interpreted the reactions governing NO_x sensing for porous YSZ based sensors and results indicated that the calculated barriers were in reasonable agreement with experiments.

