Machine Learning0Guided Screen and Design of Perovskite Oxides for High-Temperature Oxygen Sensing

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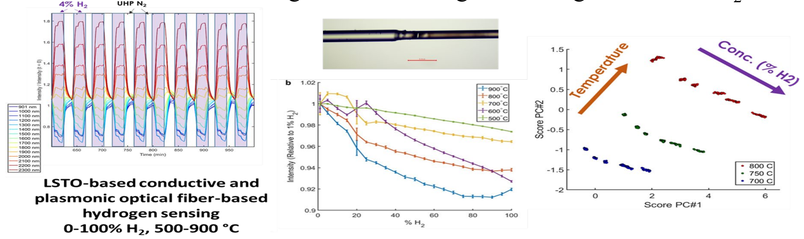
Introduction

- **For advanced real-time monitoring and control of gas species in combustion environments,** development of efficient sensing platforms and new sensor materials able to work under **harsh environments** are required.
- **Semiconducting optical-based sensor platforms** show promise. MO_x metal-oxides and ABO_3 perovskite-oxides can be attractive for high-temperature applications due to their high decomposition temperatures and structural stability; La-doped $SrTiO_3$ acts like an n-type doped semiconductor under reducing conditions – demonstrating an effective high-T sensing material for H_2.



LSTO-based conductive and plasmonic optical fiber-based hydrogen sensing
0-100% H_2, 500-900 °C

ML in Perovskite Oxide Design

1 Material Generation

- **~190 million** ABO_3 compositions: 13 A-site × 36 B-site elements
- 1-2 element with 0.7-1.0 total A/B site ratio

2 Perovskite Stability Prediction

- Gradient Boosting Classifier reduced candidates to **~40 million**
- Trained on ~1,000 verified ABO_3
- Classifier features: bond distances, Mendeleev numbers, oxidation states, and variance factors

3 Conductivity Prediction

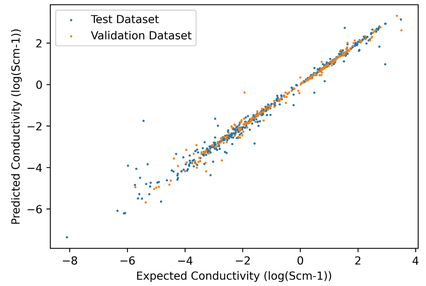
- XGBoost Regressor predicts conductivity of ABO_3 compositions, at oxygen partial pressures (pO_2) and temperatures
- Trained on over 7,000 experimental conductivity data
- Features: Magnetic moment, ionic radius, electronegativity, cell volume, band gap, formation energy, and atomic mass

4 Conductivity Sensitivity Ranking

- Identifying materials with significant conductivity changes due to oxygen partial pressure at specific temperatures ($\partial\log(\sigma)/\partial\log(pO_2)$ metric)

Conductivity Prediction

- **ML with perovskite database**
  - Priya et al trained XG boost regressor model with perovskite database of over 7,230 experiment conductivity data points across 415 unique compositions
  - 110 features derived from Materials Project & element data as well as O_2 partial pressure & temperature



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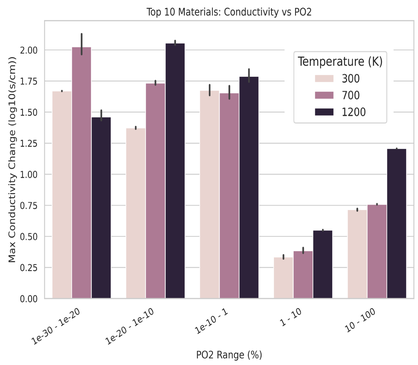
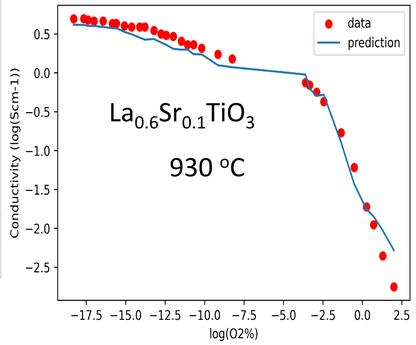
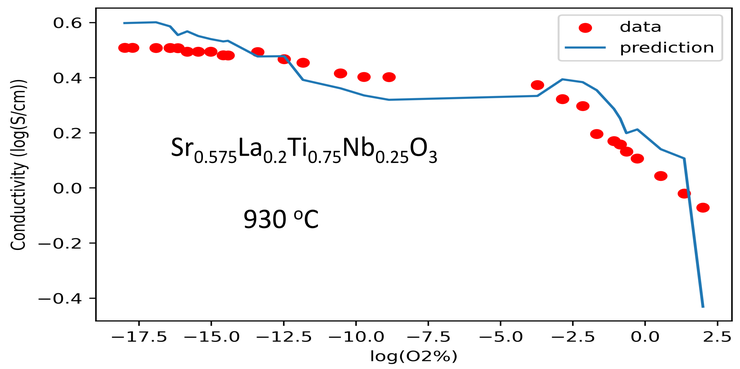
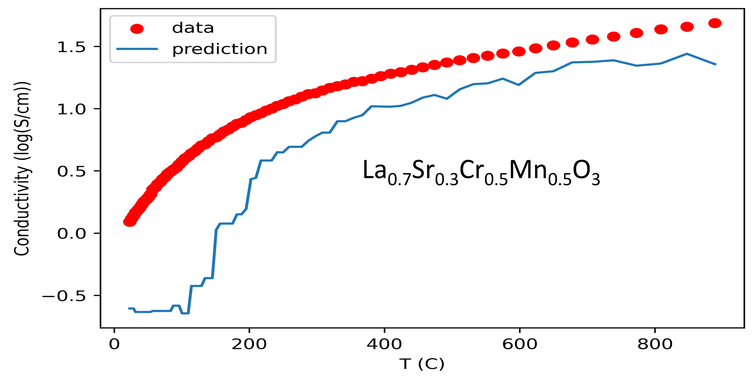




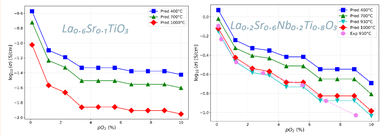




Industrial Applications

AUTOMOTIVE EXHAUST GAS MONITORING

Operating conditions: 300–1000°C | pO_2: 0.001–0.1 atm

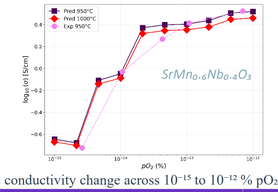


~10× conductivity change across 0.1–10% pO_2

Top 5 @ 700°C	Δ log(σ)
$La_{0.6}Sr_{0.1}TiO_3$	0.88
$La_{0.2}Sr_{0.6}Nb_{0.2}Ti_{0.8}O_3$	0.79
$La_{0.55}Sr_{0.15}Nb_{0.05}Ti_{0.95}O_3$	0.71
$La_{0.55}Sr_{0.15}TiO_3$	0.70
$La_{0.4}Sr_{0.4}TiO_3$	0.69

STEEL MANUFACTURING FURNACES

Operating conditions: 1000°C | pO_2: 10^{-17} to 10^{-14} atm

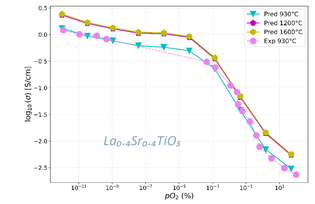


~10× conductivity change across 10^{-15} to 10^{-12} % pO_2

Top 5 @ 1000°C	Δ log(σ)
$SrMn_{0.6}Nb_{0.4}O_3$	1.13
$Ca_{0.05}Sr_{0.95}Mn_{0.6}Nb_{0.4}O_3$	1.06
$Sr_{0.8}Yb_{0.2}Mn_{0.65}Nb_{0.05}O_3$	1.05
$Sr_{0.7}Yb_{0.3}Mn_{0.65}Nb_{0.05}O_3$	1.05
$Sr_{0.85}Yb_{0.15}Mn_{0.65}Nb_{0.05}O_3$	1.04

GLASS MANUFACTURING

Operating conditions: 1200–1600°C | pO_2: 10^{-14} to 0.5 atm

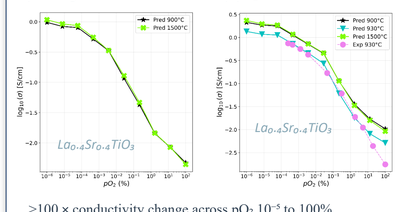


>100 × conductivity change across pO_2 (10^{-12} to 50%)

Top 5 @ 1200°C	Δ log(σ)
$La_{0.4}Sr_{0.4}TiO_3$	2.52
$La_{0.6}Sr_{0.1}TiO_3$	2.52
$La_{0.45}Sr_{0.25}TiO_3$	2.41
$La_{0.55}Sr_{0.15}TiO_3$	2.39
$Ba_{0.25}Y_{0.45}Nb_{0.05}Ti_{0.95}O_3$	2.37

SEMICONDUCTOR PROCESSING (SiC MOS)

Operating conditions: 900–1500°C | pO_2: 10^{-8} to 1 atm

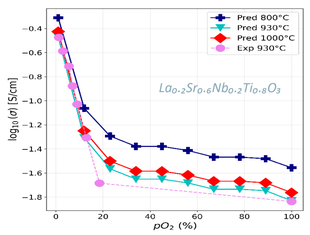


>100 × conductivity change across pO_2 10^{-5} to 100%

Top 5 @ 900°C	Δ log(σ)
$La_{0.4}Sr_{0.4}TiO_3$	2.32
$La_{0.6}Sr_{0.1}TiO_3$	2.31
$La_{0.55}Sr_{0.15}TiO_3$	2.18
$La_{0.25}Sr_{0.55}Nb_{0.15}Ti_{0.85}O_3$	2.15
$La_{0.3}Sr_{0.5}Nb_{0.15}Ti_{0.85}O_3$	2.14

Pt THIN-FILM RESISTOR PROCESSING

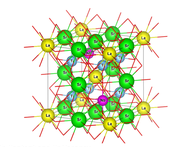
Operating conditions: 800–1000°C | pO_2: 0.01–1 atm

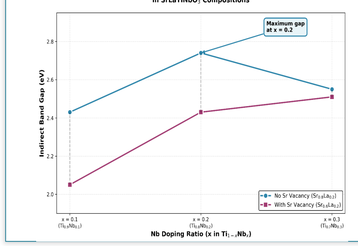


Top 5 @ 1000°C	Δ log(σ)
$La_{0.2}Sr_{0.6}Nb_{0.2}Ti_{0.8}O_3$	1.34
$Nd_{0.85}Pr_{0.15}AlO_3$	1.25
$Nd_{0.9}Pr_{0.1}AlO_3$	1.25
$Gd_{0.15}La_{0.85}AlO_3$	1.25

DFT MODELLING

$La_{0.2}Sr_{0.6}Nb_{0.2}Ti_{0.8}O_3$





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