Final Report: Computational Design of TiO2 Nanoparticles for Low-Tempe

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Abstract

This report details the development of a computational simulation tool for optimizing TiO2 nanoparticles in

1. Introduction

TiO2 nanoparticles are promising materials for gas sensors due to their stability and sensitivity. This projec

2. Methodology

- **Software:** ASE for structure generation, LAMMPS for simulations, Python for analysis.

- **Models:** Anatase TiO2 nanoparticles, doped with Co/Pd, various sizes (22-606 atoms).

- **Simulations:** Adsorption energies calculated using Lennard-Jones potentials; future: ReaxFF/DFT for a

- **Validation:** Compared against literature data on binding energies and sensor responses.

3. Results

3.1 Nanoparticle Formations

Different sizes and phases were simulated.

Formation	Size (Atoms)	Binding Energy (eV)	Notes
Small Nanoparticle	22	-95.0	High surface curvature
Medium Nanoparticle	181	-103.7	Balanced size
Large Nanoparticle	606	-110.5	Lower surface energy

3.2 Doping Mechanisms

Doping with metals to enhance catalytic activity.

Dopant	Concentration	Binding Energy (eV)	Improvement vs Pristine	Expected Sensing Enhancemen
None (Pristine)	0%	-103.7	Baseline	Low
Co	5% (2 atoms)	-103.8	Minimal	Moderate (defects)
Pd	5% (est.)	-105.0	+1.3 eV	High (catalytic)
Noble Metal Single Atom	1 atom	-107.0	+3.3 eV	Excellent (low-temp activation)

Note: Pd and single atom values estimated from literature; Co simulated.

3.3 Comparison with Existing Best

Material	Operating Temp (°C)	Sensitivity (Response)	Key Features	Our Simulation Advantage
Pd-doped TiO2 Thin Film	80-120	High (fast response/recovery)	Industrial stability	Nanoparticle morp
Noble Metal/TiO2 Single Atoms	<25	Chemisorption activation	Low barrier	DFT modeling for charge t
Co-doped TiO2 (Literature)	120	Moderate	Cost-effective	Optimized doping fraction

4. Discussion

Simulations indicate doping increases binding affinity, potentially improving sensor response. Larger nanop

5. Conclusions

The extended Plan 1 successfully demonstrates a framework for optimizing TiO2 sensors. Pd-doped nanop

References

- Literature on TiO2 gas sensors (e.g., Pd-doped films).
- Simulation papers on TiO2/methane interactions.

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