Computational Design of Aluminum Nanoparticles on Rocket Fuel using Reactive Molecular Dynamics Simulations

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Research Statement

Research Problem

Liquid fuel such as hydrocarbons, gasoline, and diesel are very common but rely on depleting resources. The major drawbacks of manufacturing hydrogen via fossil fuels:

- emission of carbon dioxide as a by-product
- shortage of fossil fuel reserves in the long term [1]

Aluminum particles can be used as a solid fuel alternative and also improve fuel efficiency. Aluminum can be the key to limited CO_2 emissions and fossil fuel usage.

Ex. of ANPs, aluminum nanoparticle dust.[10]

Importance of Aluminum

- Aluminum is the most abundant crustal metal on earth, is characterized by valuable mechanical, electrical, and thermal properties, and has low density.[1]
- Aluminum nanoparticles (ANPs) have high surface area, high reactivity, shortened ignition delays, and faster energy release.[2]

Accomplished Research

- Combustion with ethanol and ANPs, found accelerated ethanol combustion.[3]
- ANPs found to have high combustion enthalpy, low cost, and environmentally safe combustion products. As the temperature increased up to 973 K, the rate of the oxidation decreased because the diffusion paths of oxygen were blocked by the continuing oxidation process.[4]
- Metal dust oxidized by air with micron-sized aluminum droplets burning in a solid rocket motor have been analyzed.[5]
- Addition of neon and water to ANPs in combustion through molecular dynamics simulations. It was found that Ne atoms were unable to bond with the adsorbed water molecules through hydrogen-bonding, but water aids in disassociation in the oxide layer of the aluminum.[1]
- As the oxidation process continues to deform ANPs, the temperature in the system increases and by increasing the oxidizer mole fraction the temperature increases.[6,7]

Research Goal

- Most research has been conducted on aluminum microparticles or larger, where little research has been conducted on ANPs.[8] There are especially very little studies on ANPs impact with different combinations of molecules or additives.
- ANPs have the potential as a solid fuel and to improve rocket fuel, which could open doors such as further exploration in space such as Mars.[9]
- Our goal is to study the impact of ANPs in combustion with oxygen, water, and methane and its efficiency for rocket fuel via MD simulations.

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Research Methods

Computational Details

- ReaxFF reactive force field.[11]
- Reactive Molecular Dynamics (MD) Simulations. [12]
- Amsterdam Modeling Suite (AMS) software.[13]
- Using the mentioned, we are able to simulate the thermal behaviors of ANPs.

Simulation setups (4 cases)

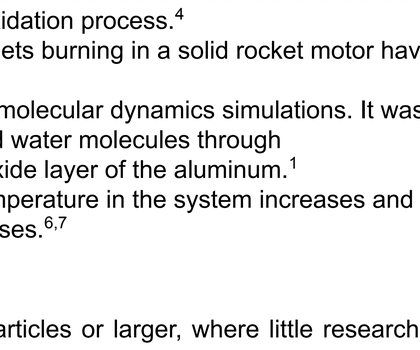
MD Simulations have been conducted for the following 4 cases:

Case 1. ANP + 650 O_2 at 400 K
a. 1,000,000 total steps: 1000 steps at 300 K, 400 K for remainder
b. Lattice 60 x 60 x 60, 1464 total atoms

Case 2. ANP + 650 O_2 at 900 K
a. 1,000,000 total steps: 1000 steps at 300 K, 900 K for remainder
b. Lattice 60 x 60 x 60, 1464 total atoms

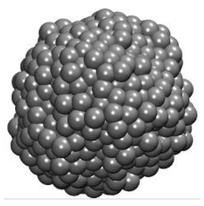
Case 3. ANP + 325 O_2 + 325 H_2O at 900 K
a. 1,000,000 total steps: 1000 steps at 300 K, 900 K for remainder
b. Lattice 48 x 48 x 48, 2489 total atoms

Case 4. ANP + 325 O_2 + 325 CH_4 at 900 K
a. 1,000,000 total steps: 1000 steps at 300 K, 900 K for remainder
b. Lattice 48 x 48 x 48, 3139 total atoms



Ex. of AMS software options

RESEARCH OBJECTIVE:
To design aluminum nanoparticles for alternative rocket fuel



: Al
: O
: C
: H

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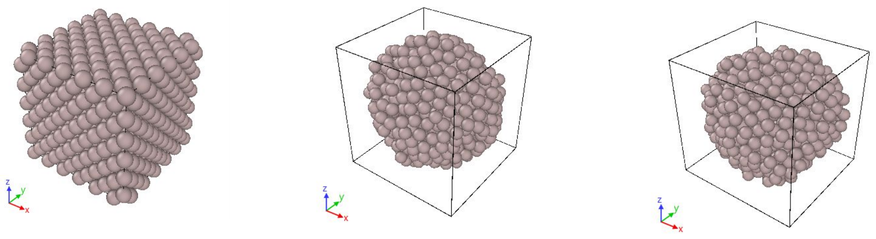
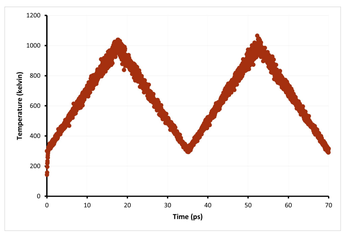
MD Result I: Designing ANPs

Al crystal (before heat treatment) | **ANP (After 1st cycle heat treatment)** | **ANP (after 2nd cycle heat treatment)**

: Al



Temperature Profile during heat treatment:



The aluminum crystal was transformed to a nanoparticle shape after the 2nd heat treatment. This will allow us to simulate more realistic nanoparticle model.`

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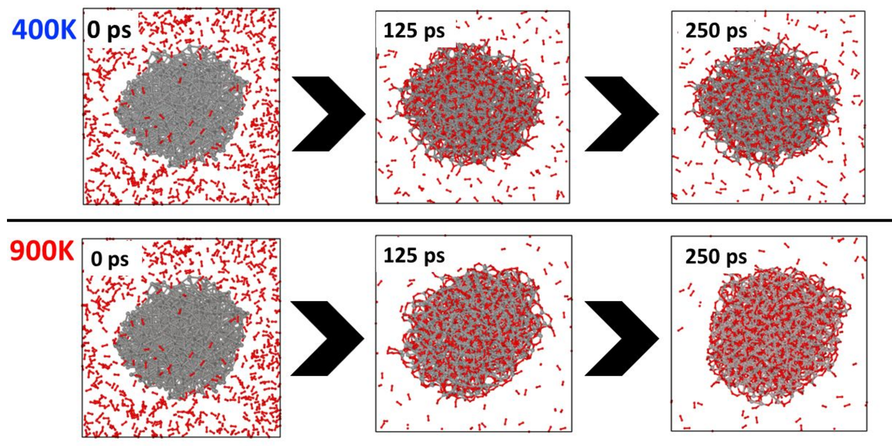
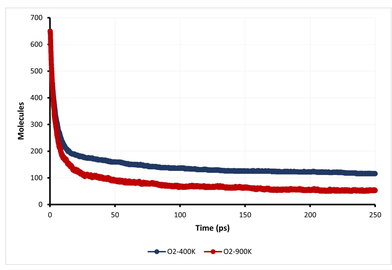
MD Results II: Burning ANPs with different Temperatures

Oxidation of ANPs by MD simulations

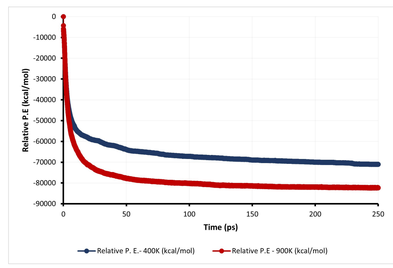
: Al : O



Number of O_2 Molecules vs Time:



Relative Potential Energy vs Time:



The 900 K simulation released more energy (almost 20,000 kcal/mol at and after 50 ps) and separated more oxygen (at least 50 more O_2 molecules) than at 400 K. So 900 K is a more effective temperature for ANP fuel and will be used in our water and methane cases.

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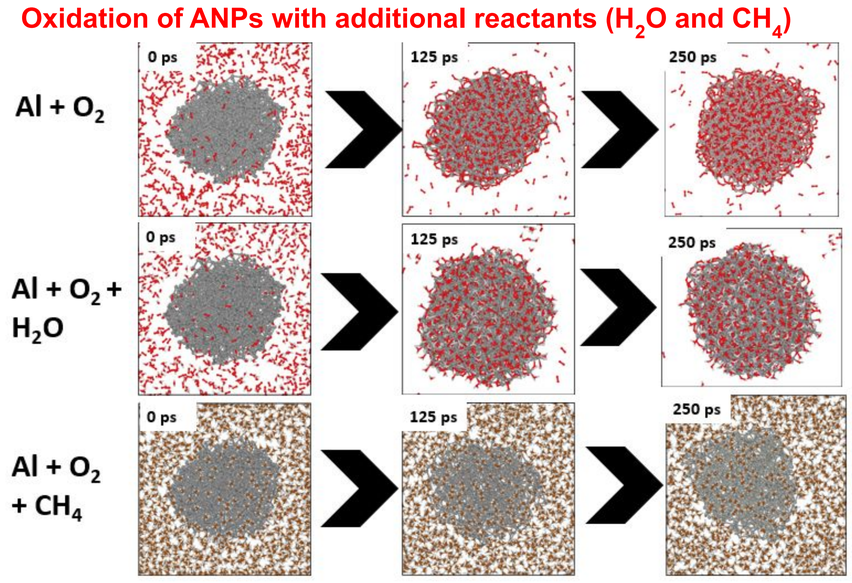
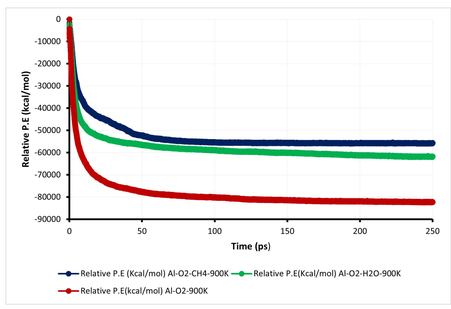
MD Results III: Burning ANPs with different reactants at 900 K

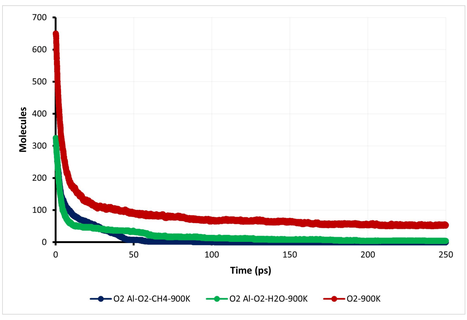
Oxidation of ANPs with additional reactants (H_2O and CH_4)



Relative Potential Energy vs Time:



Number of Molecules vs Time:



The greatest energy released from our ANP combustion MD simulations was with the oxygen at 900 K case, where the greatest access to oxygen had the best oxidation of the ANP (greatest amount of O_2 separation). Oxygen-water combustion with ANP released less energy, but released more than the combustion with oxygen-methane.

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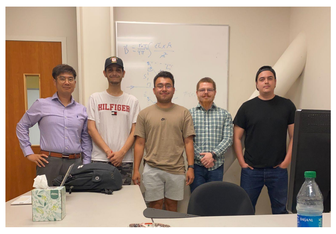
Conclusion

Our MD results revealed a fundamental understanding of ANP combustion at the atomic level. Therefore, our computational work will help guide experimental design of ANPs for the use of alternative rocket fuel.



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