**Enabling Solar Thermal Propulsion with Computational Materials Design**

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1. Background and Challenge

Solar thermal propulsion (STP) promises high specific impulse (1200 s) for missions to the interstellar medium (5x faster than Voyager):
- \( \text{H}_2 \) propellant heated up to 3500 K during close Solar approach
- Heat exchanger (HX) must survive 5 hours in hot \( \text{H}_2 \)
- Baseline uses refractory coatings to protect a carbon/carbon HX

2. Key Objectives

Use **multiscale computational techniques** to inform coating material and design by characterizing:
- Surface reactions and erosion
- Mechanical response and fracture during operation
- Integrated material response during operation

3. Coating Surface Reaction

Tungsten Case Study: Erosion occurs through surface reactions with hydrogen propellant.

- **Direct erosion**
  - Perfect surface
  - Pitted surface
  - At 2500 K: 7,500,000 times more likely than direct erosion

- **H-assisted**
  - At 2500 K: 35,000 times more likely than direct erosion

Methods include thermodynamics from quantum simulations.

4. Coating Mechanical Response and Fracture

Tungsten Case Study: Grains govern balance between plastic deformation and cracking.

5. Comparison with Heritage Operational Data

NERVA Case Study: Model observed mid-range corrosion of ZrC in hot \( \text{H}_2 \) channels to understand origins.

Erosion maximum due to carbon loss from cracks, minima are coating erosion.

6. Engagement and Forward Work

Engaged with development efforts for:
- **STP coating material selection** with JPL
- **Nuclear thermal propulsion** coatings and fuel materials material response with MSFC

Future work: Predictive modeling of fracture/crack density