1. **Research Title:** Understanding Polyimide Hygrothermal Stability via Molecular Dynamics
2. **Individual Sponsor:**

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3. **Academic Area/Field and Education Level**
Material Science, Chemistry, Physics, Computer Science with Materials Background (MS or PhD level)

4. **Objectives:**
   - **Quantify Water Absorption & Diffusion**: Model water uptake and diffusion pathways in polyimides using classical MD.
   - **Characterize Water-Polymer Interactions**: Investigate molecular interactions between water and polyimide, identifying absorption sites.
   - **Elucidate Hygrothermal Degradation**: Use ReaxFF MD to simulate and identify water-induced chemical degradation, such as hydrolysis.
   - **Correlate Molecular-Macroscopic Properties**: Link atomic-scale changes to observable macroscopic material properties.
   - **Inform Material Design**: Provide insights for designing polyimides with enhanced hygrothermal stability.
5. **Description:** Polyimides are critical high-performance polymers extensively utilized in aerospace, electronics, and other demanding applications due to their exceptional thermal stability, mechanical strength, and chemical resistance. However, their long-term performance can be significantly impacted by hygrothermal aging, where simultaneous exposure to heat and moisture leads to changes in their mechanical and chemical properties. A deeper understanding of the molecular mechanisms governing water absorption and its subsequent effects on polyimide stability is crucial for predicting their service lifetime and designing more robust materials. This proposal advocates for the use of molecular dynamics (MD) simulations, particularly with reactive force fields like ReaxFF, to model the intricate interactions between water molecules and polyimide chains. MD simulations can elucidate water ingress pathways, quantify absorption rates, and, crucially, capture potential hydrolysis reactions or other chemical changes induced by absorbed water. This approach will provide invaluable atomic-scale insights into how water compromises polyimide integrity, ultimately guiding the development of polyimides with enhanced hygrothermal stability
6. **Research Classification/Restrictions:** There are no restrictions at this time. There may be in future based on the findings.
7. **Eligible Research Institutions:** Wright State University, University of Cincinnati, Ohio State University, University of Dayton, Miami University, Ohio University
8. **PA Approval #:** AFRL-2025-3547