1. **Research Title:** Developing python-based hardware-software integration platform for closed-loop autonomous synthesis.

2. **Individual Sponsor:**

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3. **Academic Area/Field and Education Level:** Materials Science and Engineering, Chemistry, Computer Science and Engineering (Undergrad, MS, or Ph.D. level)

4. **Objectives:** Develop python based toolsets and application programming interfaces (APIs) to a) communicate with high throughput synthesis hardware ; b) develop or utilize current state of the art decision policy planning AI/ML algorithms based on characterization responses; and c) develop a graphical user interface to drive autonomous planning, executing, & decision making.

5. **Description:** While recent advancements in artificial intelligence & machine learning have led to a number of technology breakthroughs, their application in basic scientific research has only started to emerge in the past few years. In the context of synthetic organic chemistry, traditional methods often utilize previous knowledge to perform iterative experiments to identify best experimental conditions for discovering new materials, where each iteration requires significant lead time. Developing computational tool sets that can directly interact and influence reaction outcomes as well as plan future experiments by utilizing AI/ML tools, accelerates the exploration and exploitation of experimental conditions to provide optimized yields of target molecules, polymers, or particles. The project will be aimed at developing a python-based hardware-software integration platform to execute autonomous chemical reactions on an in-house AFRL platform via analytical decision making and will entail the following:

   - Developing a set of python based tool-sets or APIs that communicates with hardware to run an autonomous reaction optimization tool.
   - Developing scripts that provide decision making (policy planning via efficient exploration and exploitation of parameter space for future experiments) through analytical reasoning based on NMR and/or optical closed loop analysis.
   - Developing a graphical user interface to provide necessary inputs to drive autonomous reaction planning, executing and decision making.
   - Work closely with experimentalists to validate and iterate code to create a robust, autonomous reaction optimization tool.

6. **Research Classification/Restrictions:** This research has no ITAR restrictions.

7. **Eligible Research Institutions:** Place an X in all that apply.

   X Universities (DAGSI) X AFIT (only) USAFA

   Interest in Summer USAFA Cadet: No