1. **Research Title:** Machine Learning-Accelerated Defect Prediction in Wide Bandgap Semiconductors

2. **Individual Sponsor:**

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3. **Academic Area/Field and Education Level:** Physics, Material Science, Electrical Engineering, Electronics,/MSc or PhD

4. **Objectives:** Develop point defect predictive models based on graph neural networks informed on large first principles material science databases. This project will use existing databases that include III-V, II-VI, and group IV semiconductors, and will develop additional specialized training sets to assess the optimal dopants, doping limits and operation of silcon carbide micromechanical oscillators.

5. **Description:** Point defects in semiconductors determine their electronic, optical and mechanical properties. This project will focus on doping defects, complexes and compensating defects that can form in compound wide bandgap semiconductor lattices. The project will build an accelerated predictive platform for highly doped materials by implementing high-throughput density functional (DFT) calculations and a machine learning (ML) method based on graph neural networks. DFT has been instrumental for accurate defect formation energies, charge transition levels, diffusion barriers and carrier lifetimes. ML techniques based on neural networks offer powerful tools for rapid prediction of defect properties with DFT-accuracy by overcoming the expense of large supercells and advanced functionals. The ML algorithms used here will be trained on extensive datasets made available by leading groups for tens of thousands of configurations across the periodic table, and on specialized datasets bult in house for group IV compounds. The main application will be the design of group IV compounds with specialized elastic properties obtained by heavy doping.

6. **Research Classification/Restrictions:** Non Classified/Not Restricted

7. **Eligible Research Institutions: All**

8. **Keywords:** Wide Band Gap Semiconductors, Point Defects, First Principles, Machine Learning, Graph Neural Networks

9. **PA Approval #: AFRL-2023-4173**