

**PRF # 56067UR6**

**Project Title: iPEPICO Investigations of High-Energy Density Fuels**

**P.I. Name: Giovanni Meloni, Department of Chemistry, University of San Francisco, USA**

During the September 1, 2018 – August 31, 2019 grant period I was invited at the “35th International Symposium on Free Radicals” held in Hangzhou, China but because of my current family leave I was not able to attend the meeting and present our research. In March 2019 I travelled to the Swiss Light Source in Villigen, Switzerland for carrying out some experiments. Two projects are currently underway and we have preliminary results that we will allow us to continue to explore the investigated systems.

We published two manuscripts in journals with high impact factors:

- 1) “Reducing Properties of Superalkalis on Pyridinic Graphene Surfaces: a Computational Study,” Fabio Ramondo, Ilenia Leonzi (undergraduate student), and Giovanni Meloni,\* *ChemPhysChem* (2019) in press.
- 2) “Peroxy Self-Reaction Leading to the Formation of Furfural,” Audrey Smith (graduate student), Simone di Muzio (undergraduate student), Fabio Ramondo, and Giovanni Meloni,\* *Phys. Chem. Chem. Phys.* **21**, 10228-10237 (2019).

The “*Peroxy Self-Reaction Leading to the Formation of Furfural*” was also selected for the Journal cover. In addition, with the grant funds I paid the summer 2019 salary of two MS graduate students and two undergraduates who were able to work on their research. One of them presented one poster at the 257<sup>th</sup> ACS National Meeting in Orlando, Florida, March 31 – April 4, 2019 and is currently working on finalizing two projects. The poster title was: “*Investigation of 2,5-Dimethylfuran Oxidation Reaction Initiated by  $O(^3P)$  atoms via Synchrotron Photoionization.*” The two undergraduates presented their work as a poster, “*Investigation of Synchrotron Photoionization Oxidation of 2-Tertbutylfuran with  $O(^3P)$  at 550 & 700K,*” at the Creative Activity and Research Day at the University of San Francisco where they won the first prize as best undergraduate poster.