

**PRF # 56067UR6**

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

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During the September 1, 2017 – August 31, 2018 grant period I was invited at an international conference in Rome, “7<sup>th</sup> World Congress on Mass Spectrometry,” as a speaker and chair session. I had the opportunity to present our research at the vast and diverse mass spectrometry audience and meet some possible collaborators. The title of my talk was “Multiplexed Synchrotron Photoionization Mass Spectrometry: Characterization of Combustion and Atmospheric Reactions.” I also presented our work at the Department of Chemistry of the University of Perugia, (Italy) on April 2018 with a seminar entitled “Synchrotron Multiplexed Photoionization Mass Spectrometry Investigations of Combustion and Atmospheric Species.” We published twelve manuscripts in journals with high impact factors:

- 1) “Reduction of Carbon Dioxide with Superalkali,” Heejune Park and Giovanni Meloni,\* *Dalton Trans.* **46**, 11942-11949 (2017).
- 2) “Study of the Synchrotron Photoionization Oxidation Initiated by O(<sup>3</sup>P) of 2-Methylfuran (2MF) under Low-Temperature Conditions at 550 and 650 K,” Yasmin Fathi and Giovanni Meloni,\* *J. Phys. Chem. A* **121**, 6966-6980 (2017).
- 3) “Investigation on the Absolute and Relative Photoionization Cross Sections of Three Potential Propargylic Fuels,” Matthew Winfough and Giovanni Meloni,\* *J. Mass. Spec.* **52**, 799-808 (2017).
- 4) “Ab initio analysis on potential superbases of several hyperlithiated species: Li<sub>3</sub>F<sub>2</sub>O and Li<sub>3</sub>F<sub>2</sub>(OH)<sub>n</sub> (n = 1,2),” Matthew Winfough and Giovanni Meloni,\* *Dalton Trans.* **47**, 159-168 (2018).
- 5) “Stability of lithium substituted silyls superalkali species,” Adam Otten and Giovanni Meloni,\* *Chem. Phys. Lett.* **692**, 214-223 (2018).
- 6) “Synchrotron Photoionization Study of Furan and 2-Methylfuran Reactions with Methylidyne Radical (CH) at 298 K,” Erica Carrasco, Kenneth Smith, and Giovanni Meloni,\* *J. Phys. Chem. A* **122**, 280-291 (2018).
- 7) “Activation of dinitrogen (N<sub>2</sub>) with a superalkali species, Li<sub>3</sub>F<sub>2</sub>,” Heejune Park and Giovanni Meloni,\* *ChemPhysChem* **19**, 256-260 (2018).
- 8) “Study of low temperature chlorine atom initiated oxidation of methyl and ethyl butyrate using synchrotron photoionization TOF-mass spectrometry,” Joseph Czekner, Craig A. Taatjes, David L. Osborn, and Giovanni Meloni,\* *Phys. Chem. Chem. Phys.* **20**, 5785-5794 (2018).
- 9) “Capturing volatile organic compounds employing a superalkali,” Heejune Park and Giovanni Meloni,\* *ChemPhysChem* **19**, 2266-2271 (2018).
- 10) “Study of Methylidyne (CH and CD) Reaction with 2,5-Dimethylfuran Using Multiplexed Synchrotron Photoionization Mass Spectrometry,” Erica Carrasco and Giovanni Meloni,\* *J. Phys. Chem. A* **122**, 6118-6133 (2018).
- 11) “Investigation of Oxidation Reaction Products of 2-Phenylethanol Using Synchrotron Photoionization,” Adam Otten, Magaly Wooten, Anthony Medrano, Yasmin Fathi, and Giovanni Meloni,\* *J. Phys. Chem. A* **122**, 6789-6798 (2018).
- 12) “Computational Investigation of LiF Containing Hypersalts,” Chelsea Price, Matthew Winfough, Heejune Park, and Giovanni Meloni,\* *Dalton Trans.* **47**, 13204-13213 (2018).

One of this article, “Activation of dinitrogen (N<sub>2</sub>) with a superalkali species, Li<sub>3</sub>F<sub>2</sub>,” was also selected for the issue cover based on the very favorable comments of the reviewers. In addition, with the grant funds I paid the summer 2018 salary of three MS graduate students who were able to work on their research. Two of them presented two posters at the 255<sup>th</sup> ACS National Meeting in New Orleans, Louisiana, March 18 – 22, 2018 and are currently working on finalizing three more projects. Their poster titles were: (a) “Synchrotron Photoionization Study of Furan and 2-Methylfuran Reactions with Methylidyne Radical (CH) at 298 K;” (b) “Reduction of CO<sub>2</sub> and N<sub>2</sub> using the Li<sub>3</sub>F<sub>2</sub> superalkali.”