Selected Publications - Luís Pedro Viegas

1. **L. P. Viegas** and A. J. C. Varandas, "The $HO_2 + (H_2O)_n + O_3$ reaction: an overview and recent developments", *Eur. Phys. J. D* **70** 48-56 (2016)
   DOI: http://dx.doi.org/10.1140/epjd/e2016-60733-5

2. **L. P. Viegas** and A. J. C. Varandas, "Role of $(H_2O)_n$ $(n = 2 - 3)$ clusters on the $HO_2 + O_3$ reaction. A theoretical study", *J. Phys. Chem. B* **120** 1560-1568 (2016)
   DOI: http://dx.doi.org/10.1021/acs.jpcb.5b07691

3. **L. P. Viegas**, Diana Carolina and A. J. C. Varandas, "Mapping the HO_3 ground state potential energy surface with DFT: Can we reproduce the MRCI+Q/CBS data?", *Chem. Phys. Lett.* **620** 61-66 (2015)
   DOI: http://dx.doi.org/10.1016/j.cplett.2014.12.034

4. **L. P. Viegas** and A. J. C. Varandas, "Coupled-cluster reaction barriers of $HO_2 + H_2O + O_3$: an application of the coupled-cluster//Kohn-Sham density functional theory model chemistry", *J. Comput. Chem.* **35** 507-517 (2014)
   DOI: http://dx.doi.org/10.1002/jcc.23458

5. **L. P. Viegas** and A. J. C. Varandas, "A detailed test study of barrier heights for the $HO_2 + H_2O + O_3$ reaction with various forms of multireference perturbation theory", *J. Chem. Phys.* **136** 114312-10 (2012)
   DOI: http://dx.doi.org/10.1063/1.3695371

6. **L. P. Viegas** and A. J. C. Varandas, "Can water be a catalyst on the $HO_2 + H_2O + O_3$ reactive cluster?", *Chem. Phys.* **399** 17-22 (2012)
   DOI: http://dx.doi.org/10.1016/j.chemphys.2011.04.022

7. **L. P. Viegas**, A. Branco and A. J. C. Varandas, "How well can Kohn-Sham DFT describe the $HO_2 + O_3$ reaction?", *J. Chem. Theory Comput.* **6**, 2751-2761 (2010)
   DOI: http://dx.doi.org/10.1021/ct100364x

8. **L. P. Viegas** and A. J. C. Varandas, "The $HO_2 + O_3$ reaction: ab initio study and implications in atmospheric chemistry", *J. Chem. Theory Comput.* **6**, 412-420 (2010)
   DOI: http://dx.doi.org/10.1021/ct900370q

9. **L. P. Viegas**, A. Alijah and A. J. C. Varandas, "Accurate ab initio based multisheeted double many-body expansion potential energy surface for the three lowest electronic singlet states of H_3^+", *J. Chem. Phys.* **126**, 074309-9 (2007)
   DOI http://dx.doi.org/10.1063/1.2566770