Abstract Submitted
for the GEC20 Meeting of
The American Physical Society

Dissociative electron attachment studies of molecules containing amide bond[1] DIPAYAN CHAKRABORTY, LAUREN ECKERMANN, IAN CARMICHAEL, SYLWIA PTASINSKA, University of Notre Dame, PTASINSKA RESEARCH TEAM — Dissociative electron attachment (DEA) to biomolecules plays an important role in understanding radiation damage to biological targets initiated by high-energy radiation. The DEA studies on biological systems containing the amide bond provide the necessary information to understand their fragmentation [1-2]. Our recent study revealed that the dissociation of the amide bond in the DEA process can proceed through the core-excited Feshbach resonance, where the resonant electron capture occurred into one of the metastable valance states of the molecule. However, the resonant states' characterisation is not possible due to the complex nature of the molecules. In the present context, we focus on smaller molecules containing amide bonds, that can be considered models for larger biologically relevant molecules, i.e. peptides. Here, we present our recent experimental and computational studies of gas-phase DEA to N-ethylformamide and N-ethylacetamide molecule. The location of different resonant states and their corresponding dissociation channels are identified. With the help of quantum chemistry calculations, threshold energies of each dissociation channels are calculated. [1] J. D. Gorfinkiel and S. Ptasinska, *J. Phys. B: At. Mol. Opt. Phys.,* 2017, 50, 182001. [2] Z. Li, M. Ryszka, M. M. Dawley, I. Carmichael, K. B. Bravaya and S. Ptasinska, *Phys. Rev. Lett.,* 2019, 122, 073002.

[1]The U.S. Department of Energy Office of Science, Office of Basic Energy Sciences under Award Number DE-FC02-04ER15533.

Dipayan Chakraborty
University of Notre Dame

Date submitted: 17 Sep 2020 Electronic form version 1.4