Abstract Submitted
for the DAMOP19 Meeting of
The American Physical Society

Theoretical Studies of Dissociative Recombination of Electrons with SH^+ Ions[1] D. O. KASHINSKI[2], J. T. BOHNEMANN, United States Military Academy, A. P. HICKMAN, Lehigh University, D. TALBI, Universityé Montpellier — We are investigating the dissociative recombination (DR) of electrons with the molecular ion SH^+, i.e. $e^- + SH^+ \rightarrow S + H$. SH^+ is found in the interstellar medium (ISM), and its chemistry is still not fully understood. Understanding the role of DR of electrons with SH^+ will lead to more accurate astrophysical models. Recently we addressed the $^2\Pi$ potential energy curves (PECs) of SH as a DR pathway [3]. We are extending this work to investigate the ground and excited $^4\Pi$ PECs of SH as an alternate DR pathway. Large active-space multi-reference configuration interaction (MRCI) electronic structure calculations were performed using the GAMESS code to obtain the PECs for several values of SH separation. Rydberg-valence coupling has proven to be important. The block diagonalization method was used to disentangle interacting states and form a diabatic representation of the PECs. The status of this ongoing work will be presented at the conference.

[1]work supported by the French CNRS, the NSF, the XSEDE, and USMA
[2]travel supported by DoD-HPCMP
[3]Kashinski, Talbi, Hickman *et al.*, J. Chem. Phys. **146**, 204109 (2017)

David Kashinski
United States Military Academy

Date submitted: 01 Feb 2019 Electronic form version 1.4