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The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT

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RPPR Final Report
as of 26-Aug-2019

Agency Code:

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STEM Degrees: 0 **STEM Participants:** 0

Major Goals: The major goals of the DURIP project were to acquire dedicated computing devices to enable our group to enhance currently funded research by the DoD on ultracold chemistry and molecular ions, to contribute to projects currently proposed to the DoD in ultrafast molecular dynamics, and to increase in general our research capabilities in areas of interest to the DoD.

Accomplishments: We only recently purchased 4 dedicated nodes in the UConn High Performance Computing Cluster, which also gives us priority access to other nodes in the queue procedures of the cluster. In fact, the nodes were purchased in May, i.e. only a few months ago. Hence, no results have yet led to publications, although some preliminary results were obtained with the new equipment.

Since acquiring the equipment, we have been able to start computing Franck-Condon factor (FCF) to excite simple poly-atomic molecules in the hope to find candidates that would allow direct laser cooling, or at least allow optical detection by photon scattering. We have concentrated our effort on BaOCa+, which is a molecule considered by a member of our ARO funded MURI. Our preliminary results indicate that laser cooling might not be possible, since the FCF is 0.85: it is believed that values near 0.98 or 0.99 are required for direct laser cooling. However, a value of 0.85 would be sufficient for direct optical detection of the molecule, which would enhance drastically the experimental capabilities of our collaborators.

We also started to compute long-range interactions between poly-atomic linear neutral molecules. Again, we got only preliminary results, but they also indicate that classes of simple molecules could be aligned by external electric fields and provide interesting long-range features in the interaction potentials. We looked at Li-O-Na as a case study.

Training Opportunities: Since we just purchased the equipment, there has been few training opportunities. A new graduate student joining my group has started to use the equipment, but it is only in the initial stage.

Results Dissemination: Nothing to Report

Honors and Awards: Nothing to Report

Protocol Activity Status:

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Technology Transfer: Nothing to Report

PARTICIPANTS:

Participant Type: PD/PI
Participant: Robin Cote
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Nothing to report.