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## **Ultracold Polar Molecules: New Phases of Matter for Quantum Information and Quantum Control**

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**13. SUPPLEMENTARY NOTES**

**14. ABSTRACT**  
This "final" report is a summary of the annual work reports for grant 10-3081; two years into the grant, the PI left this institution for the University of Strasbourg, and so this grant has been terminated and superseded by grant FA8655-13-1-3032, and the work is ongoing.  
In the first two years of the project the investigators examined the use of ultracold (millikelvin to microkelvin) atoms and molecules in lattices to discover new ways of manipulating and characterizing their interactions. Notable accomplishments in the first two years include theorization of a supersolid state in ultracold polar molecules trapped in optical 2D and 1D lattices, proposition and examination of ways to obtain long-range interactions in gases of atoms weakly dressed by laser light, prediction of the existence of stable liquids/crystals of multimers (trimers, etc) of polar molecules trapped in 1D optical lattices, design of a dissipative cooling scheme for polar molecules and Rydberg atoms which could lead to cooling of polar molecules to microkelvin temperatures, and design of the first schemes for quantum information processing in self-assembled crystals of polar molecules. These accomplishments represent significant progress toward AFOSR research goals in quantum simulation and quantum information processing, and the continuation of the superseding grant should produce excellent results. The new grant was enacted with a start date of 8/1/2013, but no significant progress was made in early 2013 due to the transfer.

**15. SUBJECT TERMS**  
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Final report: grant FA8655-10-1-3081, Ultracold Polar Molecules: New Phases of Matter for Quantum Information and Quantum Control

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Report author: LtCol Victor B. Putz, AFOSR/EOARD, Project Officer

This constitutes the final report for grant FA8655-10-1-3081. During the operation of this grant, the primary investigator, Guido Pupillo, changed institutions and now is assigned to the University of Strasbourg. As such, this grant has been terminated and a new one has superseded it, grant number FA8655-13-1-3032, and the work is ongoing. As such, this final report summarizes information from the previous interim work reports for the purpose of closing out the initial grant.

## Project Goals

Ultracold atoms and molecules trapped in optical lattices provide a venue for simulation of quantum effects in much smaller subatomic particles using atoms or molecules large enough for manipulation. Understanding how to exploit the electromagnetic field control of ultracold molecules and use them to produce and characterize new phases of matter is of high interest to AFOSR and has been the goal of a recent MURI project. The Innsbruck grant aimed to bring together (i) physics of collisions of the molecules, (ii) physics of the quantum phases which could be realized with strongly interacting polar molecules, and (iii) exploration of quantum optics and quantum computing applications of polar molecules trapped in optical lattices, with an emphasis on interaction with the UMD MURI team.

## First Phase

The 2011 phase made good strides in many areas (see the 2011 annual work unit summary report, which itself is summarized here). Highlights of the 2011 progress included:

- Specific predictions for elastic and reactive rates of quasi-2D and quasi-1D collisions of reactive ultracold molecules, predicting evaporative cooling achievable in experiments; these predictions were experimentally verified by the JILA group (<http://jila.colorado.edu>).
- Determined phase diagram of ultracold polar molecules trapped in optical 2D and 1D lattices, showing the ground state of such a system can support exotic phases (supersolid) and so-called “Devil’s staircases” of lattice solids.
- Opened a line of research in the study of dipolar gases, proposing ways to obtain long-range interactions in gases of atoms weakly dressed by laser light.

The first stage of the grant focused on interdisciplinary work with the UMD MURI team and in particular PI Paul Julienne and the JILA group, with a detailed study of collision rates of molecules (finding: inelastic

collision rates can be suppressed by confining particles to 2D geometry using an optical lattice), resulting in an experiment published in Nature Physics, and spawning an effort to achieve evaporative cooling of the molecules in 2D geometry. The team then began research on a quantum computing architecture exploiting the tunable long-range dipole-dipole interactions of cold polar molecules.

#### **Summary of first-phase detailed results:**

- Showed that dipole-dipole interactions between ultracold polar molecules can be manipulated using external electric DC, enabling direct control over elastic/inelastic collisions and thus over chemical reactions in a strongly interacting molecular gas.
- Showed that a trapping configuration should also make evaporative cooling in a gas of KRb molecules technically feasible.
- Showed that a 2D optical lattice configuration will lead to the microscopic realization of Hubbard-like models with long-range interactions, possibly enabling realization of a supersolid phase.
- Using quantum Monte Carlo techniques, studied quantum phases of bosonic polar molecules on 2D square lattice interacting via repulsive dipole-dipole interactions, discovering regions where the ground state is supersolid (for finite tunneling) and in the limit of small tunneling found clear evidence for a “Devil’s staircase” where Mott solids appear at rational fillings of the lattice.
- Studied 1D fermionic and bosonic gases with repulsive power-law interactions in the framework of Tomonaga-Luttinger liquid (TLL) theory, linking the TLL parameter to the microscopic Hamiltonian.
- Studied BCS superfluid transition in single-component fermionic gas in a trap with dipole moments polarized in perpendicular layers, finding that many-body effects have a pronounced effect on critical temperature and can either decrease or increase the transition temperature.
- Discussed techniques to generate long-range interactions in a gas of ground state alkali atoms by weakly admixing excited Rydberg states with laser light, showing that residual spontaneous emission from the Rydberg state acts as a heating mechanism leading to a quantum/classical crossover.
- Used techniques developed for generating long-range interactions in a cold gas of alkali atoms to study new exotic quantum phases, predicting a supersolid phase for an ensemble of Rydberg atoms in the dipole-blockade regime—significantly, self-assembled, meaning appearing in free space even in the absence of an underlying optical lattice potential.
- Investigated formation of crystalline states with systems of polar molecules or Rydberg atoms loaded into a deep optical lattice. Using the time-evolving block decimation (TEBD) algorithm, obtained crystalline states for system sizes/parameters corresponding to reasonable experimental configurations.

## **Second Phase, 2012**

The 2012 Annual Work Unit Summary is itself summarized here. Major highlights include

- Prediction of the existence of stable liquids/crystals of multimers (trimers etc) of polar molecules trapped in 1D optical lattices
- Design of a dissipative collision scheme for polar molecules and Rydberg atoms which will lead to cooling of polar molecules to microkelvin temperatures
- First schemes for quantum information processing in self-assembled crystals of polar molecules

The cooling mechanism proposed could be used to cool polar molecules from the millikelvin to microkelvin regime, representing a significant improvement and possibly forming the basis for cooling non-alkali molecules to ultracold temperatures, and the progress toward using self-assembled crystals as quantum registers is significant progress toward the goal of realizing a quantum computer.

### Summary of second-phase detailed results

- Studied a situation where polar molecules are confined to two coupled 1D wires, showing different pairing scenarios (bound states). In particular, proved that a gas of trimers made of two particles on one wire and one on the other may be stabilized in these systems.
- Proposed/analyzed a specific scenario of engineered collisions involving laser-dressed atoms and ground-state molecules, with potentially useful properties including: strong repulsive shields to protect from inelastic collisions (and chemical reactions); large scattering cross-sections for elastic scattering between atom and molecules over a temperature range from several millikelvins down to microkelvins; design of a “dissipative collision” where a spontaneously emitted photon carries away kinetic energy of the collision partners, providing significant energy loss in a single collision—suggesting that rapid cooling of a molecule by the cold atom reservoir is possible.
- Discussed encoding of qubits into long-lived spin states of the molecular ground state, stabilized against collisions by repulsive dipole-dipole interactions. Described a new approach for implementing controlled single and two-qubit operations based on resonantly-enhanced spin-spin interactions, mediated by a localized phonon mode.
- Presented a general strategy for generating state and time dependent dipole moments to implement a universal set of gate operations for molecular qubits and analyzed the resulting gate fidelities under realistic conditions.
- Described a simple scheme for the implementation and control of spin-spin interactions in self-assembled crystals of cold polar molecules, showing that by choice of an appropriate time-dependent modulation of moments, the resulting interactions can lead to long-range tunable spin-spin interaction patterns. This can be used to generate multiparticle entangled states and spin models with long-range/frustrated interactions.
- Explored possibility for creating and detecting mesoscopic supersolids in confined Rydberg-dressed Bose-Einstein Condensates (BECs) by probing their response to forced trap rotations. Demonstrated that crystalline order and superfluidity persist at temperatures of the order of several hundreds of nanokelvins, enabling supersolid creation in cold atom experiments.

## Papers published during grant 10-3081

### 2011 Phase

- 1) F. Cinti, P. Jain, M. Boninsegni, A. Micheli, P. Zoller, and G. Pupillo, *Supersolid Droplet Crystal in a Dipole-Blockaded Gas*, Phys. Rev. Lett. **105**, 135301 (2010).
- 2) B. Capogrosso-Sansone, C. Trefzger, M. Lewenstein, P. Zoller, and G. Pupillo, *Quantum Phases of Cold Polar Molecules in 2D Optical Lattices*, Phys. Rev. Lett. **104**, 125301 (2010).
- 3) M. Dalmonte, G. Pupillo, and P. Zoller, *One-Dimensional Quantum Liquids with Power-Law Interactions: The Luttinger Staircase*, Phys. Rev. Lett. **105**, 140401 (2010).
- 4) A. Micheli, Z. Idziaszek, G. Pupillo, M. A. Baranov, P. Zoller, and P. S. Julienne, *Universal Rates for Reactive Ultracold Polar Molecules in Reduced Dimensions*, Phys. Rev. Lett. **105**, 073202 (2010).
- 5) G. Pupillo, A. Micheli, M. Boninsegni, I. Lesanovsky, and P. Zoller, *Strongly correlated gases of Rydberg-dressed atoms: quantum and classical dynamics*, Phys. Rev. Lett. **104**, 223002 (2010).
- 6) J. Schachenmayer, I. Lesanovsky, A. Micheli, and A.J. Daley, *Dynamical crystal creation with polar molecules of Rydberg atoms in optical lattices*, New J. Phys. **12**, 103044 (2010).
- 7) M. Baranov, A. Micheli, S. Ronen, and P. Zoller, *Bilayer superfluidity of fermionic polar molecules: Many-Body effects*, Phys. Rev. A **83**, 043602 (2011).

### 2012 Phase

- 1) N. Henkel, F. Cinti, P. Jain, G. Pupillo, and T. Pohl, *Supersolid vortex crystals in Rydberg-dressed Bose-Einstein condensates*, Phys. Rev. Lett. **108**, 265301 (2012).
- 2) B. Zhao, A. W. Glaetzle, G. Pupillo, and P. Zoller, *Atomic Rydberg Reservoirs for Polar Molecules*, Phys. Rev. Lett. **108**, 193007 (2012).
- 3) M. Dalmonte, P. Zoller, and G. Pupillo, *Trimer Liquids and Crystals of Polar Molecules in Coupled Wires*, Phys. Rev. Lett. **107**, 163202 (2011)
- 4) Y. L. Zhou, M. Ortner, and P. Rabl, *Long-range and frustrated spin-spin interactions in crystals of cold polar molecules*, Phys. Rev. A **84**, 052332 (2011).
- 5) M. Ortner, Y. L. Zhou, P. Rabl, P. Zoller, *Quantum information processing in self-assembled crystals of polar molecules*, Quantum Information Processing **10**, 793-819 (2011).