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| REPORT DOCUMENTATION PAGE                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |                   |                                | 2                                                    | Form Approved OMB NO. 0704-0188                          |                                                    |
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| 1. REPORT DATE (DD-MM-YYYY)<br>28-03-2014                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |                   | 2. REPORT TYPE<br>Final Report |                                                      | 3. DATES COVERED (From - To)<br>1-Oct-2011 - 31-Dec-2013 |                                                    |
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|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                   |                                | 5b. GRANT NUMBER                                     |                                                          |                                                    |
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|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                   |                                | 5d. PROJECT NUMBER                                   |                                                          |                                                    |
| 6. AUTHORS<br>Inna Ponomareva                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                   |                                | 5e. TASK NUMBER                                      |                                                          |                                                    |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                   |                                | 5f. WORK UNIT NUMBER                                 |                                                          |                                                    |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                   |                                |                                                      |                                                          |                                                    |
| 7. PERFORMING ORGANIZATION NAMES AND ADDRESSES<br>University of South Florida at St. Petersburg<br>3650 Spectrum Blvd<br>Suite 160<br>Tampa, FL 33612 -9446                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                   |                                | 8. PERFORMING ORGANIZATION REPORT NUMBER             |                                                          |                                                    |
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| 14. ABSTRACT<br>In the project we have developed computational methodology and tools to study ultrafast dynamics in ferroelectrics in bulk and nanostructure forms to simulate interaction of such materials with THz radiation. The following has been achieved: 1) development of computational methodology and tools for simulations; 2) one paper published (Nanotechnology 24, 045501 (2013)), one manuscript under consideration in Physical Review B (manuscript code BM12344), one manuscript in preparation; 3) one student graduated with B.S. in physics (GPA>3.5) and continued to PhD program at UISE, two students graduated with a master degree, one student will graduate with a                                                                                                                                                                                                                                 |                   |                                |                                                      |                                                          |                                                    |
| 15. SUBJECT TERMS<br>THz sensors, ferroelectric nanostructures, molecular dynamics, ultrafast dynamics                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                   |                                |                                                      |                                                          |                                                    |
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| a. REPORT<br>UU                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | b. ABSTRACT<br>UU | c. THIS PAGE<br>UU             |                                                      |                                                          | 19b. TELEPHONE NUMBER<br>813-974-7286              |

## Report Title

Final report on the project "Terahertz Nanoscience of Multifunctional Materials: Atomistic Exploration"

### ABSTRACT

In the project we have developed computational methodology and tools to study ultrafast dynamics in ferroelectrics in bulk and nanostructure forms to simulate interaction of such materials with THz radiation. The following has been achieved: 1) development of computational methodology and tools for simulations; 2) one paper published (Nanotechnology 24, 045501 (2013)), one manuscript under consideration in Physical Review B (manuscript code BM12344), one manuscript in preparation; 3) one student graduated with B.S. in physics (GPA>3.5) and continued to PhD program at USF, two students graduated with a master degree, one student will graduate with a PhD in physics in summer 2014.

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**Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:**

**(a) Papers published in peer-reviewed journals (N/A for none)**

| <u>Received</u> | <u>Paper</u>                                                                                                                                                                |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 08/22/2013 2.00 | R Herchig, Kimberly Schultz, Kevin McCash, I Ponomareva. Terahertz sensing using ferroelectric nanowires , Nanotechnology, (02 2013): 0. doi: 10.1088/0957-4484/24/4/045501 |
| <b>TOTAL:</b>   | <b>1</b>                                                                                                                                                                    |

Number of Papers published in peer-reviewed journals:

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**(b) Papers published in non-peer-reviewed journals (N/A for none)**

| <u>Received</u> | <u>Paper</u> |
|-----------------|--------------|
| <b>TOTAL:</b>   |              |

Number of Papers published in non peer-reviewed journals:

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**(c) Presentations**

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**Non Peer-Reviewed Conference Proceeding publications (other than abstracts):**

Received      Paper

**TOTAL:**

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**Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):**


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**Peer-Reviewed Conference Proceeding publications (other than abstracts):**

Received      Paper

**TOTAL:**

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**Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):**


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**(d) Manuscripts**

Received      Paper

|            |      |                                                                                                                                                                                                       |
|------------|------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 03/26/2014 | 4.00 | Kevin McCash, B. K. Mani, C.-M. Chang, and I. Ponomareva. The role of mechanical boundary conditions in the soft mode dynamics of PbTiO <sub>3</sub> ,<br>( )                                         |
| 08/07/2012 | 1.00 | R. Herchig, Kimberly Schultz, Kevin McCash, I. Ponomareva. Terahertz nanosensing using ferroelectric nanowires,<br>Applied Physics Letters (under consideration) (07 2012)                            |
| 08/30/2013 | 3.00 | Kevin McCash, B. K. Mani,, C.-M. Chang,, and I. Ponomareva. The role of mechanical boundary conditions on the soft modedynamics in PbTiO <sub>3</sub> ,<br>To be submitted for publication. (09 2013) |

**TOTAL:      3**

Books

Received

Paper

TOTAL:

Patents Submitted

Patents Awarded

Awards

Inna Ponomareva received outstanding (early) tenure and promotion in 2013;  
Inna Ponomareva received outstanding faculty award in 2014.

Graduate Students

| NAME            | PERCENT SUPPORTED | Discipline |
|-----------------|-------------------|------------|
| Kevin McCash    | 0.50              |            |
| James Almand    | 0.16              |            |
| FTE Equivalent: | 0.66              |            |
| Total Number:   | 2                 |            |

Names of Post Doctorates

| NAME            | PERCENT SUPPORTED |
|-----------------|-------------------|
| Chun-Min Chang  | 0.30              |
| FTE Equivalent: | 0.30              |
| Total Number:   | 1                 |

Names of Faculty Supported

| NAME            | PERCENT SUPPORTED | National Academy Member |
|-----------------|-------------------|-------------------------|
| Inna Ponomareva | 0.10              |                         |
| FTE Equivalent: | 0.10              |                         |
| Total Number:   | 1                 |                         |

Names of Under Graduate students supported

| NAME            | PERCENT SUPPORTED | Discipline |
|-----------------|-------------------|------------|
| Ryan Herchig    | 0.20              | Physics    |
| FTE Equivalent: | 0.20              |            |
| Total Number:   | 1                 |            |

### Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: ..... 1.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 1.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 1.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 1.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense ..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: ..... 0.00

### Names of Personnel receiving masters degrees

NAME

James Almand, 2013

Kevin McCash, 2012

**Total Number:** 2

### Names of personnel receiving PHDs

NAME

Kevin McCash, summer 2014 expects

**Total Number:** 1

### Names of other research staff

NAME

PERCENT SUPPORTED

**FTE Equivalent:**

**Total Number:**

### Sub Contractors (DD882)

### Inventions (DD882)

### Scientific Progress

see attachment

### Technology Transfer

# Final report for the project “Terahertz nanoscience of multifunctional materials: atomistic exploration”

PI: *Inna Ponomareva*

We have accomplished the following.

1. We have developed a set of computational tools to simulate interaction of THz radiation with ferroelectrics in bulk and nanoforms. In particular, we developed a fast molecular dynamics simulator that can be used for simulations of both isothermal and isentropic processes.

2. We have developed parametrization of force field for ferroelectric  $\text{BaTiO}_3$  that accurately reproduces the dynamical properties of this material in tetragonal phase.

3. We have proposed an original approach to sense THz radiation using ferroelectric nanowires. A thermodynamical model has been developed to describe interaction of ferroelectric nanowires with THz radiation. The study has been published in *Nanotechnology* 24, 045501 (2013) [impact factor 3.842].

2. We have developed and used a fast molecular dynamics simulator to study the soft mode dynamics of bulk ferroelectric  $\text{PbTiO}_3$  under hydrostatic pressure and biaxial strains. This study is significant in multiple ways. First of all, it is a first comprehensive study on the role of mechanical boundary conditions in the soft mode dynamics. Secondly, it establishes the existence of Curie-Weiss stress and strain laws. Thirdly, it offers a way to uniquely identify the mechanical boundary conditions associated with different ferroelectric nanostructures by the change in the soft mode frequencies. The manuscript is under consideration in *Physical Review B* (BM12344).

3. We have discovered a novel way to control the polarization direction in ferroelectric nanowires by application of THz pulses. Such approach is based on application of tailored time-dependent electric field. More precisely, a bias *dc* electric field of sub-switching strength is applied to the nanowire along the direction opposite to that of the polarization. The field is not sufficient to reverse the polarization. At a later time the simulated sample is subjected to a THz Gaussian pulse of an electric field. The interaction of the pulse with the nanowire results in the energy dissipation and increase in the temperature. As a result the free-energy landscape changes lowering the energy barrier for the polarization reversal. Under the new conditions the bias field is sufficient to reverse the polarization. Fig.1 provides the results of our first-principles-based simulations and demonstrates the polarization reversal through application of the electric-field pulse.

The effect is robust and occurs under conditions when the frequency of the electric field in the pulse is comparable to the intrinsic frequency of the soft mode. The manuscript is being finalized for publication.

4. The project supported (partially) one undergraduate student who has graduated with BS degree in Physics and continued to PhD studies at USF. Two students partially supported by the project have obtained Master Degree in Applied Physics. One student partially supported by the project will graduate with PhD degree in Applied Physics in May 2014.

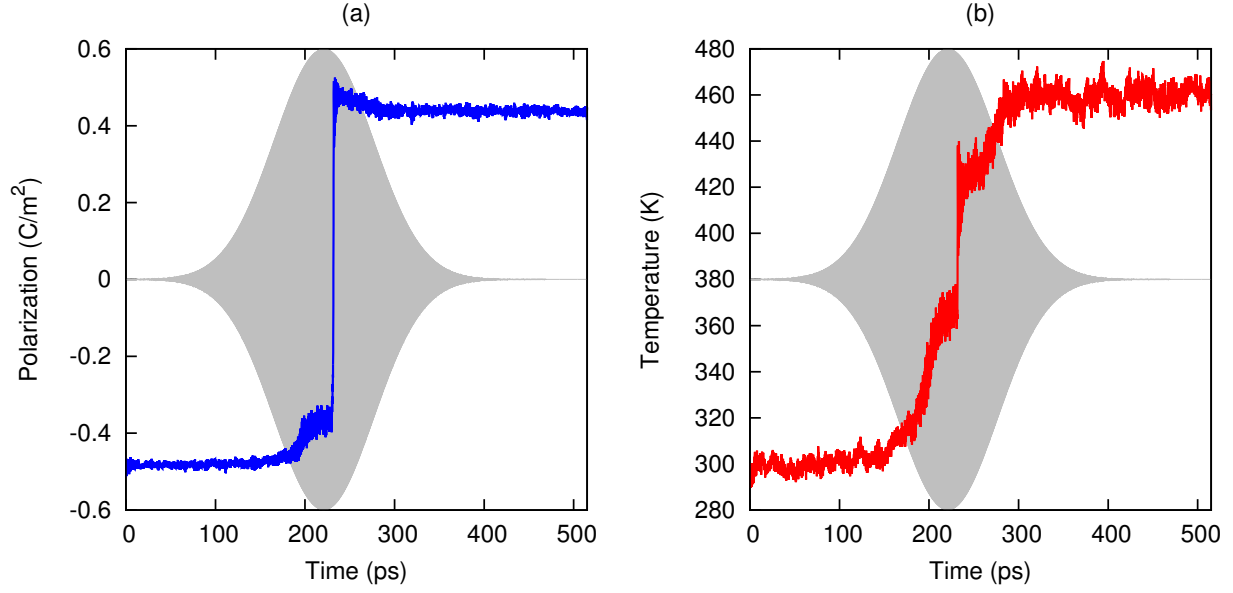


FIG. 1. The time evolution of the polarization (a) and temperature (b) in a PbTiO<sub>3</sub> nanowire as obtained from first-principles-based simulations. The grey shading outlines the electric field in the THz pulse given by the equation  $E = E_0 \cos(\omega t) \exp\left(-\left(\frac{t-t_0}{\tau}\right)^2\right)$ . The bias field in the simulations is 50% of the switching field, while the amplitude of the field in the pulse,  $E_0$ , is 20% of the switching field.