

### INTRODUCTION

We summarize the achievements of our research group by discussing individual projects, list of publications in peer-reviewed scientific journals, poster presentations at conferences, seminars, tutorials, and special courses. Among our goals are: to understand mechanisms involved into the processes of energy transfer at molecular level (including biological systems) and to propose and simulate the behavior of new type of nanoscale devices. All our algorithms were prepared on the basis of physical models, while high-fidelity simulations were performed on multi-core computers.

### Faculty Mentors



**Dr. Kamil Walczak**  
Assistant Professor  
Team Leader, NYC  
(Quantum Transport)



**Dr. Uday Sukhatme**  
Professor, Provost  
Lecturer, NYC  
(Supersymmetry)



**Dr. Mohsen Shiri-Garakani**  
Associate Professor  
Lecturer, PLV  
(Quantum Spacetime)

### Dr. Walczak's Research Group

**Omar Tsoutiev**, major: Mathematics | 2017 – 2018  
Project: “Thermal and Shot Noises in Quantum-Interference Devices”

**Hunter Tonn**, major: Chemistry | 2017 – 2018  
Project: “Heat Transfer Controlled by Quantum Interference Effects”

**Joanna Dyrkacz**, major: Biology | 2015 – 2018  
Project: “Inelastic Heat Transport in Molecular Complexes”

**Erica Butts**, major: Biology | 2016 – 2017  
Project: “Transport Phenomena in Memristive Neuronal Networks”

**David Saroka**, major: Physics, Mathematics | 2015 – 2017  
Project: “Tunneling of Heat: Analysis of Nonlinear Transport Regime”

**Rita Aghjayan**, major: Biology, minor: Physics | 2014 – 2017  
Project: “Thermal Rectification and Transients in Correlated Systems”

**Arthur Luniewski**, major: Biology, minor: Physics | 2014 – 2017  
Project: “Molecular Noise and High-Intensity Heat Fluxes at Nanoscale”

**Luke Shapiro**, major: Biochemistry | 2015 – 2016  
Project: “Memristive Characteristics of Nanoscale Thermal Devices”

### List of Publications

**Walczak, K.**; and Saroka, D.: “*Tunneling of Heat: Beyond Linear Response Regime.*” *Physica E*, Vol. 96, pp. 57-61 (2018).

Luniewski, A.; and Aghjayan, R.; and **Walczak, K.**: “*Nonlinearities and Noise-Signal Relations in Electronic Heat Transport via Molecules.*” arXiv:1601.06712 (2016); Manuscript Accepted (2017) .

**Walczak, K.**: “*Nanoscale Heat Conduction: Modeling Prospects.*” Dekker Encyclopedia of Nanoscience and Nanotechnology, 3rd Ed. (2016).

Lekawa-Raus, A.; **Walczak, K.**; Kozlowski, G.; Hopkins, S.; Wozniak, M.; Glowacki, B.; Koziol, K.: “*Low temperature electrical transport in modified carbon nanotube fibres.*” *Scripta Materialia*, Vol. 106, pp. 34-37 (2015).

Lekawa-Raus, A.; **Walczak, K.**; Kozlowski, G.; Wozniak, M.; Hopkins, S.; Koziol, K.: “*Resistance-temperature dependence in carbon nanotube fibres.*” *Carbon*, Vol. 84, pp. 118-123 (2015).

### Poster Presentations (Selected)

Tsoutiev, O.; and **Walczak, K.** (2018, March 6) “*Thermal and Shot Noises Generated by Hot Electrons in Quantum-Interference Devices.*” APS March Meeting 2018, Los Angeles, CA.

Tonn, H.; and **Walczak, K.** (2018, March 6) “*Hopping-type Modifications of Quantum Interference Conditions in Nanoscale Thermal Junctions.*” APS March Meeting 2018, Los Angeles, CA.

**Walczak, K.** (2018, February 5) “*The Ground-State Wave Function of The Universe Closed In A Bubble.*” Dr. Walczak's Group Meeting, Pace University, New York City, NY.

**Walczak, K.** (2018, January 12) “*Hückel Molecular Orbitals for Aromatic and Unsaturated Hydrocarbons.*” Dr. Walczak's Group Meeting, Pace University, New York City, NY.

**Walczak, K.** (2018, January 3) “*Hydrogenic Schrödinger Orbitals.*” Dr. Walczak's Group Meeting, Pace University, New York City, NY.

**Walczak, K.** (2017, December 21) “*Density Functional Theory In A Nutshell.*” Dr. Walczak's Group Meeting, Pace University, New York, NY.

**Walczak, K.** (2017, December 19) “*Fundamentals of DFT Bandstructure Calculations of Defect-Free Materials.*” Dr. Walczak's Group Meeting, Pace University, New York City, NY.

**Walczak, K.** (2017, October 25) “*Qubit-Accompanied Quantum Fluxes in Closed Nanosystems.*” Presidential Inauguration Day, Pace University, New York City, NY.

Tonn, H.; and **Walczak, K.** (2017, October 25) “*Thermal Transport Properties of Quantum-Interference Devices.*” Presidential Inauguration Day, Pace University, New York City, NY.

Butts, E.; and **Walczak, K.** (2017, May 4) “*Quantum Correlations in Transport via Memristive Neuronal Networks.*” Pace University Research Day 2017, New York City, NY.

Saroka, D.; **Walczak, K.** (2017, May 4) “*Tunneling of Heat: Beyond Linear Response Regime.*” Pace University Research Day 2017, New York City, NY.

**Walczak, K.** (2017, May 4) “*Nonlinearities and Noise-Signal Relations in Phononic Heat Transfer via Molecules.*” Pace University Research Day 2017, New York City, NY.

Butts, E.; and **Walczak, K.** (2017, May 4) “*Ion Channel Memristors (ICMs) as Logical Transistors.*” Pace University Research Day 2017, New York, NY.

Dyrkacz, J. N.; **Walczak, K.** (2017, March 14) “*Electron-Phonon Coupling Effects in Molecular Heat Conduction.*” APS March Meeting 2017, New Orleans, LA. (May 4) Pace University Research Day 2017, New York, NY.

Saroka, D.; and **Walczak, K.** (2016, March 16) “*Tunneling of Heat: Potential-Barrier Analysis.*” APS March Meeting 2016, Baltimore, MD.

**Walczak, K.** (2016, March 16) “*Nonlinear Transport and Noise Properties of Acoustic Phonons.*” APS March Meeting 2016, Baltimore, MD.

Dyrkacz, J. N.; **Walczak, K.** (2016, March 16) “*Inelastic Heat Transfer in Molecular Quantum Dots.*” APS March Meeting 2016, Baltimore, MD. (May 3) Pace University, Student and Faculty Research Day 2016, New York, NY.

Aghjayan, R.; Luniewski, A.; **Walczak, K.** (2015, March 5) “*Transient Heat Conduction in Strongly Correlated Systems.*” APS March Meeting 2015, San Antonio, TX. (April 22) Pace University Research Day 2015, New York, NY.

Luniewski, A.; Aghjayan, R.; **Walczak, K.** (2015, March 5) “*Nonlinearities and Noise Properties of Electronic Heat Transfer in Molecular Junctions.*” APS March Meeting 2015, San Antonio, TX. (2015, April 22) Pace University Research Day 2015, New York City, NY.

### Works in Progress (Selected)

**Walczak, K.**: “*Quantum Fluxes Generated and Modified by Qubit Dynamics.*” Invited Chapter in Encyclopedia; In Press.

**Walczak, K.**: “*Relativistic Quantum Energy Flux in Post-Fourier Heat Transport Equations.*” In Press.

**Walczak, K.**; Aghjayan, R.; and Luniewski, A.: “*Thermal Rectification and Relaxation Processes in Strongly Correlated Systems.*” In Press.

**Walczak, K.**: “*First-Principles Approach to Transfer of Energy and Momentum in Quantum Systems.*” Manuscript in Preparation.

**Walczak, K.**: “*Nonlinear Transport and Noise Properties of Acoustic Phonons.*” Manuscript in Preparation.

Dyrkacz, J. N.; and **Walczak, K.**: “*Inelastic Heat Conduction via Molecular Systems.*” Manuscript in Preparation.

### Seminars and Tutorials (Selected)

**Walczak, K.** (2018, January 5) “*Evolution of Spin in Electromagnetic Fields and Pauli Wave Equations.*” Dr. Walczak's Group Meeting, Pace University, New York City, NY.

**Walczak, K.** (2018, January 2) “*Deuteron and Dihydrogen Cation: Toward Many-Particle Quantum Systems.*” Dr. Walczak's Group Meeting, Pace University, New York City, NY.

**Walczak, K.** (2017, December 28) “*Helium Atom: Variational Treatment and Perturbative Approach.*” Dr. Walczak's Group Meeting, Pace University, New York City, NY.

**Walczak, K.** (2017, December 5) “*Beyond Hartree: A Quest for Sufficient Treatment of Electron Correlations.*” Dr. Walczak's Group Meeting, Pace University, New York City, NY.

**Walczak, K.** (2017, November 14) “*A Pedestrian's Guide to DFT Calculations.*” – A Tutorial for Students. Dr. Walczak's Group Meeting, Pace University, New York City, NY.

**Walczak, K.** (2017, November 7) “*Intro to Bandstructure Theory of Solids.*” – A Tutorial for Students. Dr. Walczak's Group Meeting, Pace University, New York City, NY.

**Walczak, K.** (2017, October 31) “*A Gentle Intro to Tight-Binding Modeling.*” – A Tutorial for Students. Dr. Walczak's Group Meeting, Pace University, New York City, NY.

**Walczak, K.** (2017, May 23) “*Schrödinger Equations and Quantum Fluxes.*” Dr. Walczak's Group Meeting, Pace University, New York, NY.

**Walczak, K.** (2017, May 17) “*Quantum Transport Theory: New Perspectives.*” Dr. Walczak's Group Meeting, Pace University, New York City, NY.

Aghjayan, R.; and **Walczak, K.** (2017, March 14) “*Transient Heat Effects at Nanoscale.*” APS March Meeting 2017, New Orleans, LA.

Shapiro, L.; **Walczak, K.** (2016, March 16) “*Thermal Memristive Devices.*” APS March Meeting 2016, Baltimore, MD.

**Walczak, K.**; and Yerkes, K. L. (2015, March 4) “*First-Principles Approach to Transient Heat Flow in Quantum Systems.*” APS March Meeting 2015, San Antonio, TX.

### Courses Developed by Dr. Walczak

**PHY 395** (2014-2018) – Special lectures on Thermal Physics and Quantum Transport with integrated computer lab.

**BIO 395** (2016-2018) – Special lectures on Quantum Biology and Energy Conversion with integrated computer lab.