

National Institute of Physics

Management Team

Terminal Report for the Structure and Dynamics Research Program

Period covered: 01 January 2019 to 31 December 2019

Prepared by:

Ronald S. Banzon, PhD. (August to December 2019)

and Cristine D. Villagonzalo, Dr. rer. nat. (January to July 2019)

Program Coordinators

Structure and Dynamics Research Program

Submitted: 23 March 2020

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1 Executive Summary

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1.1.2 Mentoring

Degree Program	Sem 2 AY 17–18 (p. 4)	Midyear 2018	Sem 1 AY 18–19 (p. 5)	Total
BS Physics	3	0	1	4
BS Applied Physics	6	0	0	6
MS Physics	0	0	0	0
Total	9	0	1	10

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2 Technical Report

2.1 Activities of the Research Program

In 2019 nine students graduated and completed their theses in SanD. SanD membership (faculty and students) is now 45 and the research group is reaching full capacity. The group had 2 international peer reviewed articles and 19 local conference peer-reviewed papers. One of the highlights of this calendar year is the continued activity of SanD faculty in organizing and supporting the activities of the Samahang Pisika ng Pilipinas and in strengthening the linkages with node members of the Asian Network in Condensed Matter and Complex Systems.

2.1.1 Organization

Regular Members (3)

- 1) Villagonzalo, Cristine – Professor
- 2) Banzon, Ronald – Associate Professor
- 3) Paraan, Francis – Associate Professor

PhD Student Members (6)

- 1) Ilano, Neris – D10
- 2) Villegas, Vladimir D6
- 3) Cortez, April – D4
- 4) dela Rosa, Rafael – D4, University Research Associate 1 (URA 1)
- 5) Itable, Gene Moses – D4
- 6) Acosta, Geronimo Allan Jerome – D3

MS Student Members (7)

- 1) Ayang-ang, Cleofe Dennielle – M2
- 2) Mangada, Mykhal – M6
- 3) Guinid, Jammy Rey – M4, URA 1 (from 1 Jan. 2019 - 31 July 2019)
- 4) Masbate, Julius – M4
- 5) Elegado, Christopher Patrick – M1
- 6) Esperanza, Robertson – M2
- 7) Tan, Apolinario Miguel – M2

BS Student Members (19)

- 1) Dumanjog, Mignon Francis – B6
- 2) Urbano, Kryss – B6
- 3) Adelino, Joanne Mae – B5
- 4) Castro, Marc Jerrone – B5
- 5) Co, Richmond – B5
- 6) Deleon, Monica Cecilia – B5
- 7) Delima, Krishna Lyn – B5
- 8) Go, Mary Chris – B5
- 9) Gomez, Jacob – B5
- 10) Ramos, Aaron Paul – B5
- 11) Ancheta, Sheenah – B5

- 12) Bunagan, Marc Jason – B5
- 13) Calpatura, Jairus Carlo – B4
- 14) De Guzman, Tristan – B5
- 15) Edora, Maria Alena – B4
- 16) Estrada, John Benedick – B4
- 17) Ganding, Jersey Dianne – B4
- 18) Rodriguez, Tim Jeff – B4
- 19) Sacres, Kobe Brian – B4

Apprentices (3)

- 1) Accad, Vincent Rhey – M1
- 2) Dimacali, Raphael Angelo – B3
- 3) Maddumba, Marc Lesney – B3

2.1.2 Mentoring

Graduated Sem 2 AY 2018–2019

BS Physics (3)

- 1) Narag, Dean Von Johari C.
BS Thesis: Effects of Tensile and Compression Strain on The Electronic Structure of Free-Standing Silicene Using the Density Functional Theory
Adviser: Cristine Villagonzalo
- 2) Mactal, Gerard Antonio L.
BS Thesis: Modelling the Anomalous Diffusion of Tracer Particles on a Graphene Lattice Using Random Walks and Site Percolation
Adviser: Cristine Villagonzalo
- 3) Villano, Celso Jr. T.
BS Thesis: Monte Carlo Approach to Epithelial Cell Proliferation Along a One-Dimensional Axis
Adviser: Cristine Villagonzalo

BS Applied Physics (Instrumentation) (5)

- 1) De Leon, Kryzz Joshua G.
BS Thesis: Tensor Flow Implementation of Singular Value Decomposition in the Density Matrix Renormalization Group
Adviser: Francis Paraan
- 2) Go, Michael Nicholas
BS Thesis: Deterination of the Higher Order Periods of The Logistic Equation Using A Chebyshev Transform
Adviser: Ronald Banzon
- 3) Lopez, Vidal Wyatt M.
BS Thesis: Effects of Image Preprocessing on the Supervised Classification of Radiographs
Adviser: Francis Paraan
- 4) Medrano, Matthew
BS Thesis: Computational Fluid Dynamics Analysis of Lift and Drag on the Teardrop 2.0 and Towpedo Submersible
Adviser: Francis Paraan

5) Rivera, Vincent S.

BS Thesis: Fidelity of a 4-Bit Grover's Quantum Search Algorithm Application in an Ising Spin System with Limited Precision

Adviser: Ronald Banzon

BS Applied Physics (Materials Physics) (1)

1) Ongkiko, Mario

BS Thesis: Density Functional Theory Study of Small Molecule Adsorption on Graphene

Adviser: Francis Paraan

Graduated Sem 1 AY 2019–2020

BS Physics (1)

1) Urbano, Kryss

BS Thesis: Effect of Region Size Without Spin in a 2D Ising System

Adviser: Ronald Banzon

2.2 Research Highlights**2.2.1 International peer-reviewed articles (2)**

- 1) Santos-Putungan, Alexandra B., Stojic, Natasa, Binggeli, Nadia & Francis N.C. Paraan. 2019. "Strong chemisorption of CO₂ on B₁₀-B₁₃ planar-type clusters." *Journal of Physics: Condensed Matter* **31**, 145504. DOI: [10.1088/1361-648x/aafabd](https://doi.org/10.1088/1361-648x/aafabd).
- 2) Chiong, Meliton III, & Francis N.C. Paraan. 2019. "Controlling the nucleophilic properties of cobalt salen complexes for carbon dioxide capture." *Royal Society of Chemistry Advances* **9**, 23254. DOI: [10.1039/C9RA01990A](https://doi.org/10.1039/C9RA01990A).

2.2.2 International conference presentations (2)

- 1) Ayang-ang, CDP, & FNC Paraan. Quantum Phase Transitions and Schmidt Gap Closing in a Kitaev Chain with Long-Ranged Interactions, in the 19th Asian Quantum Information Science (AQIS) Conference Abstract Booklet - Poster Day 1, 174 - 175 (Korea Institute for Advanced Study, Seoul, 2019).
- 2) Esperanza, RC & FNC Paraan. Ground State Entanglement in an Extended Hubbard Model with Ising-like Interactions, in the 19th Asian Quantum Information Science (AQIS) Conference Abstract Booklet - Poster Day 1, 164 (Korea Institute for Advanced Study, Seoul, 2019).

2.2.3 Local peer-reviewed conference papers (19)

- 1) Narag, Dean Von Johari C. & Cristine Villagonzalo. Investigation on the effect of tensile and compressive strain on the electronic structure of silicene using the density functional theory, in the Proceedings of the 37th Samahang Pisika ng Pilipinas Physics Conference, SPP-2019-PA-16 (Tagbilaran City, Philippines, 2019).
- 2) Ongkiko, Mario Antonio T. & Francis N.C. Paraan. Molecular projected band structure of ammonia and ammonium adsorbed on graphene, in the Proceedings of the 37th Samahang Pisika ng Pilipinas Physics Conference, SPP-2019-PA-17 (Tagbilaran City, Philippines, 2019).
- 3) Go, Mary Chris R. & Francis N.C. Paraan. Classification of chest radiographs using depthwise separable convolution, in the Proceedings of the 37th Samahang Pisika ng Pilipinas Physics Conference, SPP-2019-PA-21 (Tagbilaran City, Philippines, 2019).

- 4) Lopez, Vidal Wyatt M. & Francis N.C. Paraan. Image preprocessing with bi-histogram equalization in a supervised classification of radiographs, in the Proceedings of the 37th Samahang Pisika ng Pilipinas Physics Conference, SPP-2019-PA-22 (Tagbilaran City, Philippines, 2019).
- 5) Adelino, Joanne Mae B. & Ronald S. Banzon. Implementation of a quantum algorithm for solving linear equations, in the Proceedings of the 37th Samahang Pisika ng Pilipinas Physics Conference, SPP-2019-PB-10 (Tagbilaran City, Philippines, 2019).
- 6) Go, Michael Nicholas R. & Ronald S. Banzon. Determining higher order periods of the Logistic equation using a Chebyshev Transform, in the Proceedings of the 37th Samahang Pisika ng Pilipinas Physics Conference, SPP-2019-PB-12 (Tagbilaran City, Philippines, 2019).
- 7) de Leon, Kryzz Joshua G. & Francis N. C. Paraan. Parallel acceleration of density matrix renormalization group calculations with TensorFlow, in the Proceedings of the 37th Samahang Pisika ng Pilipinas Physics Conference, SPP-2019-PB-14 (Tagbilaran City, Philippines, 2019).
- 8) Mactal, Gerard Antonio L. & Cristine Villagonzalo. Effects of spatial disorder in modelling the anomalous diffusion of tracer particles on a graphene lattice, in the Proceedings of the 37th Samahang Pisika ng Pilipinas Physics Conference, SPP-2019-PB-18 (Tagbilaran City, Philippines, 2019).
- 9) Gomez, Jacob M. & Francis N.C. Paraan. Evaporation and compaction of colliding dust clusters at different impact parameters, in the Proceedings of the 37th Samahang Pisika ng Pilipinas Physics Conference, SPP-2019-PB-21 (Tagbilaran City, Philippines, 2019).
- 10) Guinid, Jammy Rey C. & Ronald S. Banzon. Diversity in iteroparous Penna Model with delayed mutations, in the Proceedings of the 37th Samahang Pisika ng Pilipinas Physics Conference, SPP-2019-PB-23 (Tagbilaran City, Philippines, 2019).
- 11) Rivera, Vincent S. & Ronald S. Banzon. Floating point representation error propagation analysis in quantum computing from a fixed point example, in the Proceedings of the 37th Samahang Pisika ng Pilipinas Physics Conference, SPP-2019-PB-25 (Tagbilaran City, Philippines, 2019).
- 12) Acosta, Geronimo Allan Jerome G. & Cristine D. Villagonzalo. Current amplification and rectification in a chain of four spins individually coupled to different heat baths, in the Proceedings of the 37th Samahang Pisika ng Pilipinas Physics Conference, SPP-2019-PB-33 (Tagbilaran City, Philippines, 2019).
- 13) Delima, Krishna Lyn & Cristine D. Villagonzalo. Interlayer and intralayer interaction in a graphene junction beyond nearest neighbors, in the Proceedings of the 37th Samahang Pisika ng Pilipinas Physics Conference, SPP-2019-PB-34 (Tagbilaran City, Philippines, 2019).
- 14) Villano, Celso T. & Cristine D. Villagonzalo. Monte Carlo approach to one-dimensional cell proliferation within a tissue-cell population, in the Proceedings of the 37th Samahang Pisika ng Pilipinas Physics Conference, SPP-2019-PB-35 (Tagbilaran City, Philippines, 2019).
- 15) Co, Richmond L. & Cristine D. Villagonzalo. Simulation of continuous-time random walks with anharmonicity, in the Proceedings of the 37th Samahang Pisika ng Pilipinas Physics Conference, SPP-2019-PB-48 (Tagbilaran City, Philippines, 2019).
- 16) Medrano, Matthew R. & Francis N. C. Paraan. Computational fluid dynamics analysis of downforce and drag generated by an accessory flat plate wing on the Teardrop 2.0, in the Proceedings of the 37th Samahang Pisika ng Pilipinas Physics Conference, SPP-2019-PB-35 (Tagbilaran City, Philippines, 2019).
- 17) Castro, Marc J. R. & Francis N. C. Paraan. Multi-class semantic segmentation and volume calculation of cardiac CT scans using convolutional neural networks, in the Proceedings of the 37th Samahang Pisika ng Pilipinas Physics Conference, SPP-2019-1C-07 (Tagbilaran City, Philippines, 2019).

- 18) Urbano, Kryss C. & Ronald S. Banzon. 2D Ising model with regions without spin, in the Proceedings of the 37th Samahang Pisika ng Pilipinas Physics Conference, SPP-2019-1G-04 (Tagbilaran City, Philippines, 2019).
- 19) Esperanza, Robertson C. & Francis N. C. Paraan. Critical scaling at the Neel transition in an extended Hubbard model with Ising-like interaction, in the Proceedings of the 37th Samahang Pisika ng Pilipinas Physics Conference, SPP-2019-1G-05 (Tagbilaran City, Philippines, 2019).

2.2.4 Local conference presentations (0)

2.2.5 NIP funded projects (3)

- 1) Project Leader: Banzon, Ronald S.
Project Title: Effect of long periods between mutations in a Penna Model
Period: 01 January 2019–31 December 2019
- 2) Project Leader: Paraan, Francis Norman C.
Project Title: Scaling Exponents at Quantum Critical Points of One-Dimensional Systems
Period: 01 January 2019–31 December 2019
- 3) Project Leader: Villagonzalo, Cristine DLR.
Project Title: Stochastic Modelling of Cancer Cell Growth Using the Monte Carlo Method
Period: 01 January 2019–31 December 2019

2.2.6 Non-NIP funded projects (1)

- 1) Project Leader: Paraan, Francis Norman C.
Type: OVPAA ECWRG 2018-1-009
Project Title: Computational and theoretical studies of small molecule binding on nanoclusters and surfaces
Period: 17 September 2018 – 16 March 2020
Amount: P500 000

2.2.7 Other invited lectures/talks (0)

2.2.8 Outbound travel abroad (1)

- 1) Name: Villagonzalo, Cristine
Activity: The 21st General Council Meeting of the Asia Pacific Center for Theoretical Physics (APCTP)
Purpose: International Representation for NRCP in APCTP (as substitute for Dr. Jose Perico Esguerra, APCTP General Council Member)
Place: APCTP, Pohang, South Korea
Dates: 21-22 March 2019
Mode of exchange: Asia Pacific Center for Theoretical Physics (APCTP)

2.2.9 Inbound visiting researchers (1)

- 1) Visitor: Jayson Cosme
Affiliation: Center for Optical Quantum Technologies, Universitaet Hamburg
Purpose: Invited Seminar Talk
Title of Talk: *Dynamical Control of Phases In An Atom-Cavity System*

Duration: April 22 2019

NIP Contact: Francis Paraan

2.3 Extension Work Highlights

2.3.1 Extension Work Activities¹ (8)

- 1) Name: Francis Paraan
Extension work: Editor in Chief and Online Journal Manager
Organization: Samahang Pisika ng Pilipinas
- 2) Name: Francis Paraan
Extension work: Web Administration of <http://www.spp-online.org> and sub-domains
Organization: Samahang Pisika ng Pilipinas
- 3) Name: Francis Paraan
Extension work: Program Committee Member
Asian Quantum Information Science Conference AQIS 2019, <http://aqis-conf.org/2019/committees/>
Dates: 19-23 August 2019, Korea Institute for Advanced Study
- 4) Name: Francis Paraan
Position: Local Organizing Committee Member
Activity: Asian Network School and Workshop on Complex Condensed Matter Systems 2019
Dates: 4 November – 8 November 2019
- 5) Name: Cristine Villagonzalo
Extension work: Topical Editor
Organization: Samahang Pisika ng Pilipinas
- 6) Name: Cristine Villagonzalo
Position: Physics Division (Division IX) Chair
Organization: National Research Council of the Philippines, Governing Board
- 7) Name: Cristine Villagonzalo
Position: Network Node Coordinator for the Philippines
Organization: ICTP Asian Network on Condensed Matter and Complex Systems
- 8) Name: Cristine Villagonzalo
Position: Local Organizing Committee Co-Chair
Activity: Asian Network School and Workshop on Complex Condensed Matter Systems 2019
Dates: 4 November – 8 November 2019

2.3.2 Research Interns and Trainees (9)

- 1) Intern/Trainee: Briones, Dominic Angelo
School: PSHS Central Mindanao Campus
NIP Contact: Cristine Villagonzalo/ Francis Paraan
Dates: 10 June – 28 June 2019
Remarks: NIP PSHS Science Immersion Program (MOU)
- 2) Intern/Trainee: Cimeni, Chiara Jo Mari
School: PSHS Central Mindanao Campus
NIP Contact: Cristine Villagonzalo/ Francis Paraan
Dates: 10 June – 28 June 2019

¹From the 2003 UP Diliman Faculty Manual 2003 Section 4.3.4: Extension includes services utilizing expertise and talent related to one's discipline, outside instruction and research, such as nondegree training, seminars, workshops, conferences, review classes [except UP College Admission Test (UPCAT)], advisory/technical/information services, exhibits, performances, consultancies (without professional fee), networking, advocacy, and volunteer/community work.

- Remarks: NIP PSHS Science Immersion Program (MOU)
- 3) Intern/Trainee: Macumbal, Mohammad Azzam Rakin
School: PSHS Central Mindanao Campus
NIP Contact: Cristine Villagonzalo/ Francis Paraan
Dates: 10 June – 28 June 2019
Remarks: NIP PSHS Science Immersion Program (MOU)
- 4) Intern/Trainee: Bisochon, Jamme Omar
School: PSHS CALABARZON Region Campus
NIP Contact: Cristine Villagonzalo/ Francis Paraan
Dates: 10 June – 28 June 2019
Remarks: NIP PSHS Science Immersion Program (MOU)
- 5) Intern/Trainee: Garcia, Erdel Jerimiah
School: PSHS Cagayan Valley Campus
NIP Contact: Cristine Villagonzalo/ Francis Paraan
Dates: 10 June – 28 June 2019
Remarks: NIP PSHS Science Immersion Program (MOU)
- 6) Intern/Trainee: Adelino, Joanne Mae
School: University of the Philippines Diliman
NIP Training Supervisor: Ronald Banzon, Cristine Villagonzalo
Dates: 4 June – 30 July 2019
Remarks: DOST-SEI Summer Practical Training Program
- 7) Intern/Trainee: Ancheta, Sheenah
School: University of the Philippines Diliman
NIP Training Supervisor: Cristine Villagonzalo
Dates: 4 June – 30 July 2019
Remarks: DOST-SEI Summer Practical Training Program
- 8) Intern/Trainee: Bunagan, Marc Jason
School: University of the Philippines Diliman
NIP Training Supervisor: Francis Paraan, Cristine Villagonzalo
Dates: 4 June – 30 July 2019
Remarks: DOST-SEI Summer Practical Training Program
- 9) Intern/Trainee: Gomez, Jacob
School: University of the Philippines Diliman
NIP Training Supervisor: Francis Paraan, Cristine Villagonzalo
Dates: 4 June – 30 July 2019
Remarks: DOST-SEI Summer Practical Training Program

2.4 Challenges Encountered

- 1) Repair of the floor-type airconditioning unit did not push through. The Commission on Audit did not approve the repair through a service center as the cost exceeded 30% of the original purchase price of the unit.
Proposed solution: To request the purchase of a new airconditioning unit which will be up to standard of the 2020 new refrigerant regulations using no freon (HCFC-22) in the unit.

2.5 Awards, Accreditations, and Positions of Responsibilities Held

2.5.1 National awards and positions held (1)

- 1) Name: Francis Paraan
Position: SPP Councilor, Editor-in-Chief
Organization: Samahang Pisika ng Pilipinas

2.5.2 International awards and positions

- 1) Name: Ayang-ang, Cleofe Dennielle P.
Award: 3rd prize, Best Student Poster Award during the 19th Asian Quantum Information Science (AQIS) Conference (August 2019)
Award-giving body: AQIS 2019 Program Committee, Seoul, Korea
- 2) Name: Go, Mary Chris
Award: Outstanding Performance Award for Best Research during the 2019 MOST GASE Summer Program on Quantum Technology + Artificial Intelligence (June 2019)
Award-giving body: Taiwanese Ministry of Science and Technology Center for Global Affairs and Science Engagement, Taipei, Taiwan

3 Appendices

3.1 Photographs



SanD members, alumni and family (December 2019).