ADVANCERIT
Reimagining our Careers and Campus Culture

***Connect* Grant AY 2018**

Project Title: **Building the foundations for a computational materials-research nucleus at RIT**

PI Name: Poornima Padmanabhan Co-PI Name(s): Patricia Taboada-Serrano

1. Executive summary

The long-term vision driving the project is to position RIT as a computational-materials research hub in the academic sphere. The first step to achieve this vision is to build a nucleus of current RIT researchers working on computational materials with a shared network of collaborators, mentors and means to access external resources and visibility. The Department of Chemical Engineering in KGCOE will serve as the starting point of the nucleus. Expected impact of the project includes: (a) increased capability of recruitment of faculty in the area, (b) increased recruitment success of graduate students, and (c) increased success in garnering resources for research efforts at RIT, including funding and access to state-of-the art external facilities.

2. Project Description

Background:

Research-active faculty in the Chemical Engineering Department housed in KGCOE face unique challenges. This department has a small number of faculty with limited resources, leading to off-balance teaching and service workloads. The department currently offers only one undergraduate degree, which limits access to graduate students.[1] Disparate areas of expertise and non-overlapping research fields lead to isolated efforts in grant writing, student training and dissemination of research results. Combined, these challenges are daunting, and pose difficulties in the following areas:

(a) recruitment, hiring, and retaining of new faculty, and means towards cluster hires
(b) tools and environment leading tenure-track faculty towards a successful tenure process
(c) tools and environment leading tenured faculty towards promotion and career advancement

Proposed work:

The long-term vision driving the proposed work is to position RIT as a computational materials research hub. Such a reputation will attract human capital (faculty, graduate students and postdocs), provide a structure for faculty to develop successful careers towards tenure and promotion, and enable collaborative grant writing within RIT and in partnership with external institutions.

The PIs propose to utilize a *Connect* grant in order to put in place systems and practices that will build a research nucleus and enable its growth and sustainability long-term. The starting point for the nucleus is the Department of Chemical Engineering, with the two PIs as initiators. Both PIs work in synergistic areas of computational-materials research, spanning the spectrum from soft materials to hard-solid interfaces.

The overarching goal of the proposed project is to build a computational-materials research nucleus starting at the Chemical Engineering Department at RIT. The proposed work has the following objectives:

(a) develop a shared network of mentors and collaborators to create research opportunities in terms of applications to research funding and joint research projects

[1] The average time required for new faculty to recruit PhD students into their research groups has been over two years since the date they joined, at the Department of Chemical Engineering during the past seven years.

(b) improve visibility of the PIs, the research nucleus, and the department in the computational-materials research community

The objectives and proposed work directly benefit the advancement of the careers of the two women faculty involved in the grant, while simultaneously creating the practices, network and connectivity structure to foster the careers of other faculty at RIT involved in computational-materials research. Furthermore, the proposed activities will create conduits not only to recruit students and faculty, but also to access funding and external state-of-the-art facilities via collaborations. The expected impacts of the proposed project align perfectly with the goals of the *Connect* grants and Advance RIT, stated as follows: "*encourage leadership and career development, mentoring, networking and research collaboration, while enhancing and advancing the university's multifaceted initiatives and scholarship infrastructure*".

3. Project plan and activities

Project Mentor And Role – Dr. Jennifer Chayes: The co-PI and Dr. Chayes served together in the National Academies Committee for Women in Science, Engineering, and Medicine. Dr. Chayes started a collaborative, east-coast-wide research cluster for Microsoft. The research nucleus will benefit from her experience and expertise in establishing, growing and branding a research cluster.

The activities A through E described below pursue both objectives simultaneously.

A. Semi-monthly meetings of research nucleus within RIT:

The PIs will hold semi-monthly meetings to share information, plan and work on the activities proposed in the plan of work. These meetings will also be used to have Skype or phone meetings with the project mentor on a periodical basis. New hires in the department, whose research aligns with the nucleus, will be invited to attend meetings, and included in all networking activities. Symposia by invited speakers will enable the PIs to identify other researchers at RIT that would benefit from the research nucleus.

B. Visit to RIT of **four** invited speakers:

Invited speakers were selected keeping in mind that they could serve not only as potential collaborators but also as mentors for the alternate faculty within the nucleus. The PIs have established individual relationships with a subset of the speakers as part of current projects or scholarship efforts. The goal is to further these relationships into the submission of grants and to include individuals into the shared network of mentors and potential collaborators of the group.

C. Visit of PIs to **three** identified collaborators:

The PIs request support for work visits to identified collaborators in order to develop and submit joint funding grants. The submissions of these grants will involve the generation of preliminary data within a common project, and the establishment of a concrete plan of work for the next 3 to 5 years with these collaborators. Furthermore, the collaborative work initiated by each of the PIs will involve these collaborators with the research nucleus creating potential mentoring and work opportunities for other members of the nucleus.

Figure 1 depicts the schematic of the current (black) and desired (red) of the mentoring/collaboration network of the research nucleus. The research nucleus shown in the blue bubble comprises the two PIs and potential new hires in Chemical Engineering.

D. Travel of PIs to **two** strategic conferences:

The PIs are currently members of the Computational Molecular Science and Engineering Forum (CoMSEF) of the American Institute of Chemical Engineers (AIChE) and regularly present research work and attend events in that forum. The PIs have identified two venues specific to each of their areas of expertise within computational materials research that would expand the reach of the research nucleus. These venues include: (a) 5th International Soft-matter conference, and (b) the 93rd American

Chemical Society Colloids and Surface Science Symposium. These two conferences cover the two extremes of materials development: soft materials and hard interfaces.

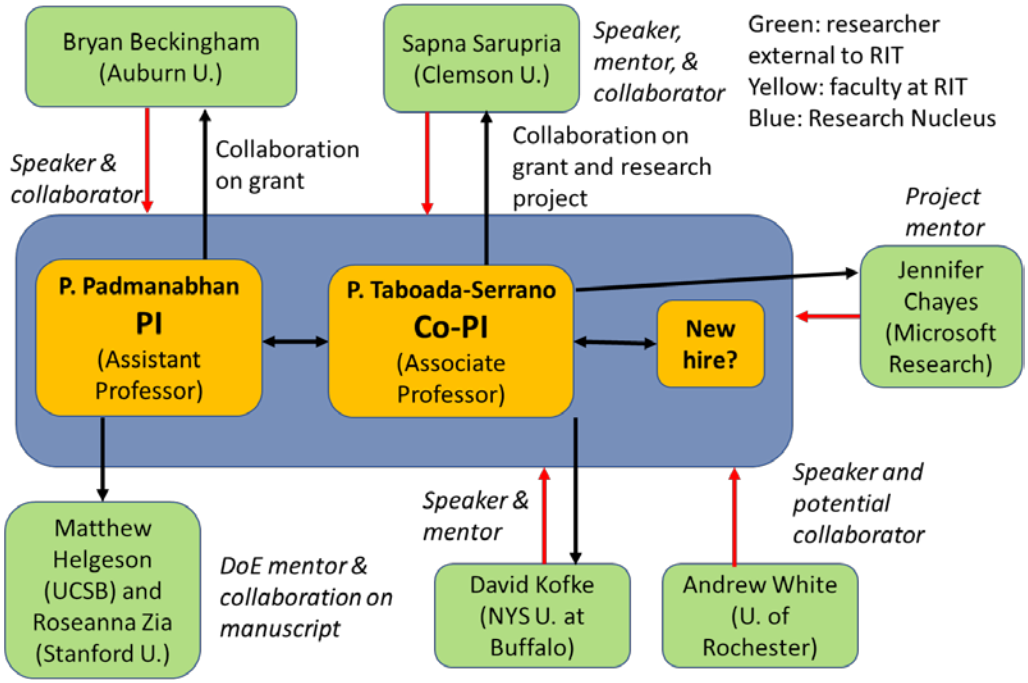

Figure 1. Schematic of the mentoring/collaboration network of the proposed research nucleus.

E. <u>Dissemination of best practices in establishing the nucleus in **two** newsletters</u>

The above activities proposed by the PIs will lay a strong foundation of a research nucleus at RIT. Lessons learned and best practices of setting up such a nucleus will be disseminated in newsletters reaching a broad audience. The PIs have identified two newsletters. The first one is published by CoMSEF on a quarterly basis, and reaches the chemical engineering and computational materials communities. The second one is published by the Association of Computing Machinery-Women every month, and reaches a global audience including industry partners, academic communities, and laypersons interested in computing. The PI has previously published her experiences in leading an outreach event organized by graduate women in chemical engineering in this venue.

4. Timeline for proposed activities

Figure 2 presents the outline for the proposed project.

Project Activities	A	M	J	J	A	S	O	N	D	J	F	M
1. Semi-monthly meetings of research nucleus within RIT												
2. Visit to RIT of four invited speakers												
3. Visit of PIs to three identified collaborators												
4. Travel of PIs to two strategic conferences												
5. Newsletters on experience and best practices in the building of a research nucleus												

Figure 2. Project timeline, outcomes and deliverables.

5. Evaluation Plan

The evaluation of the project will be performed by the completion of the activities on the period depicted by the outline. The instruments to evaluate the levels of success in achieving the stated objectives will be as follows:

- Half-page minutes on bimonthly Skype meetings with external mentor, Dr. Jennifer Chayes.
- One-page summary of collaboration visits that includes plan of action
- Seminar announcements and the speaker schedule for invitied speakers, and minutes from resulting mentorship discussions during these visits
- Conference abstracts, program booklet, and any other positive outcomes arising from the conference
- Dissemination of the research nucleus activities in the ACM-W and AIChE CoMSEF newsletters.

6. Role of project participants and relevance to their plan of work

Project Mentor – Dr. Jennifer Chayes: See Section 3 for description.

PI – Dr. Poornima Padmanabhan: The PI has established relationships with two experimental collaborators, Prof. Bryan Beckingham of Auburn University and Prof. Matthew Helgeson at University of California Santa Barbara. Collaborations between experimentalists and the PI's theoretical strengths enhance the chances of success in securing external sponsorship. The proposed activities will improve the collaborative relationship, which is the foundation for applying to a multi-million dollar grant at the Materials Genome Initiative due in 2021. Prof. Helgeson is chosen to be mentor of the PI for his expertise in non-equilibrium materials behavior, which is the only area of soft-matter research funded by the Department of Energy's Early Career Research program. Under the PI's plan of work, she will submit an application in 2020.

Co-PI – Dr. Patricia Taboada-Serrano: The co-PI has started a collaboration with Prof. Sapna Sarupria, in modelling gas hydrates at the atomic length scale. Additionally, Prof. Sarupria serves as programming chair of CoMSEF, a subdivision of AIChE, which is the home division for computational materials research in Chemical Engineering. Prof. David Kofke at University of Buffalo is currently a member of the Chemical Engineering Department advisory board and has given valuable advice to the co-PI over the past several years. Prof. Kofke is a leader in the development of algorithms for molecular simulation and serves on the editorial board for the journal Molecular Physics. The proposed activities will allow the co-PI to access funding opportunities within collaborative projects. Co-PI's CV appears as an addendum to the proposal.

8. Budget table

Dollar Amount	**Title: NSF ADVANCE *Connect* Grant Budget Template**	
X,XXX	All Travel*	
	Total Costs	$ X,XXX

Detailed budget justification write-up appears as an Addendum to the proposal.

9. How this project is relevant to the AdvanceRIT mission

The expected impacts of the proposed project align perfectly with the goals of the *Connect* grants and Advance RIT, stated as follows: "*encourage leadership and career development, mentoring, networking and research collaboration, while enhancing and advancing the university's multifaceted initiatives and scholarship infrastructure*".

10. Broader impact

A significant anticipated outcome is the successful promotion of the PIs. The proposed conferences and a majority of collaboration trips of the PI will occur prior to the submission of the mid-tenure review package in December 2019. The new collaborations and plans for funding will strengthen the case of the PI during the mid-tenure process and eventual tenure process. The co-PI will use these opportunities identified in the proposal to expand her collaboration network towards preparing a strong case for promotion to the rank of full professor. Additionally, a new faculty focused in computational research has recently accepted the offer in the department of chemical engineering and will be included in the regular meetings of the research nucleus and mentorship activities with invited speakers.

The broader impact of the proposal lies in the creation of a sustainable, high-visibility research cluster, and a marketable "brand" for RIT, that creates opportunities for growth of existing and new faculty hires. As a small and relatively new department, our bandwidth in recruiting graudate students is limited by individual efforts of the current faculty in reaching out and recruiting students. With the establishment of the research nucleus and the shared networks, we will be able to direct a concerted effort in recruiting students under this research nucleus. The research nucleus will foster joint collaborations and advising of graduate students. Together, our activities will grow our department, improve the department rankings in the broader chemical engineering community, and make us competitive in recruiting talented faculty.

11. Intellectual merit

The intellectual merit of the proposal lies in the use of two faculty members in a small department as the anchors for a research nucleus in the area of computational-materials research. By combining individual networks and identifying common sources of funding and research collaborations, the PIs are devising a new **shared mentorship-collaboration model** that can help faculty success in small departments with limited resources.

Addendum 1: Budget justification

The budget requested is itemized per type of activity in the tables below. Costs were estimated using websites and following RIT travel policies.

CONFERENCE TRAVEL			
Type of Expense	Cost ($)	Quantity	Comments
Registration	XXX	2	PIs present work in one strategic conference each
Flights: Domestic International	 XXX XXXX	 1 1	One conference is in the US the other one is in Edinburgh, Scotland.
Lodging: Domestic International	 XXX/night XXX/night	 4 nights 5 nights	
Per diem: Domestic International	 XX/day XX/day	 5 days 6 days	Conferences are weeklong, entailing 5 days of participation

COLLABORATION TRIPS			
Type of Expense	Cost ($)	Quantity	Comments
Flights	XXX	3	Flights are to small airports within the U.S.
Lodging	XXX/night	6 nights	
Per diem	XX/day	9 days	

GUEST SPEAKERS			
Type of Expense	Cost ($)	Quantity	Comments
Flights	XXX	2	Two speakers flying in, other two at driving distance to RIT. Flights covered by the Department of Chemical Engineering (see Recommendation Letter for commitment from Department Head)
Lodging	XXX/night	2 nights	Covered by the Department of Chemical Engineering (see Recommendation Letter for commitment from Department Head)
Dinner	XXX	4	

Total expenses of proposed activities: $XX,XXX.

Expenses borne by the Department of Chemical Engineering: $X,XXX.

Budget requested from the *Connect* grant: $X,XXX

Addendum 2: CV of co-PI

PATRICIA TABOADA-SERRANO, Ph.D.
Department of Chemical Engineering
Rochester Institute of Technology

Professional Experience

Jul. 2018 – Present	Associate Professor and Founding Faculty — Department of Chemical Engineering, Rochester Institute of Technology, Rochester, NY
Aug. 2011 – Jun. 2018	Assistant Professor and Founding Faculty — Department of Chemical Engineering, Rochester Institute of Technology, Rochester, NY
Jan. 2009 – Dec. 2010	Projects Manager – Alalay Foundation and UNICEF partnership, La Paz, Cochabamba and Santa Cruz, BOLIVIA Visiting Adjunct Professor – Universidad Católica Boliviana San Pablo, La Paz, BOLIVIA
Jan. 2006 – Aug. 2008	Post-doctoral Research Associate – Oak Ridge National Laboratory, Oak Ridge, TN
Jan. 1996 – Dec. 1998	Research and Development Engineer – Centro de Ciencias Aplicadas, La Paz, BOLIVIA

Education and Training

Jan. 2006 – Aug. 2008	Post-doctoral Research Associate — Oak Ridge National Laboratory, Oak Ridge, TN
Aug. 2001 – Dec. 2015	Ph.D. in Environmental Engineering – Georgia Institute of Technology, Atlanta, GA
Jan. 1999 – Jul. 2001	M.Sc. in Chemical Engineering – Universidad Simón Bolívar, Caracas, VENEZUELA
Jan. 1991 – Dec. 1995	B.S. in Chemical Engineering – Universidad Mayor de San Andrés, La Paz, BOLIVIA

Awards and Honors

- *2004 Molecular Design Institute Fellow*, Office of Naval Research – U.S. Department of Defense.
- *2001 – 2003 Fulbright Fellow*, U.S. Department of State (The Fulbright Fellowship is awarded to one person in Bolivia per year)

Professional Activities

- Member of the American Institute of Chemical Engineers, The American Chemical Society and the American Association for the Advancement of Science

Selected Publications

- Li, X. Pustullka, S., Pedu, S., Close, T., Xue, Y., Richter, C., Taboada-Serrano, P. Titanium dioxide nanotubes as model system for electrosorption studies, Nanomaterials 2018, 8:404-.
- Ney, E., Hou, C.-H., Taboada-Serrano, P. "Electrical double layer potential inside nanopores from Classic Electrodynamics and Grand Canonical Monte Carlo simulations", J. Chem.Eng. Data 2018, 63:2557-2566.
- Li, X.; Close, T.; Pustulka, S.; Pedu, S.; Xue, Y.; Richter, C.; Taboada-Serrano, P. "Electrosorption of monovalent alkaline metal ions onto mesoporous titanium dioxide nanotubes", Electrochimica Acta, 2017, 231:632-640.
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- Walker, M.E.; McFarlane, J.; Glasgow, D.C.; Chung, E.; Taboada-Serrano, P.; Yiacoumi, S.; Tsouris, C. "Influence of radioactivity on surface interaction forces", Journal of Colloid and Interface Science, 2010, 350:595.

- Taboada-Serrano, P.; Ulrich, S.; Szymcek, P.; McCallum, S.; Phelps, T. J.; Palumbo, A.; Tsouris, C. "A multi-phase, micro-dispersion reactor for the continuous production of methane gas hydrate", Ind. Eng. Chem. Res. 2009, 48:6448.
- Hou, C.-H.; Taboada-Serrano, P.; Yiacoumi, S.; Tsouris, C. "Monte Carlo simulation of electrosorption selectivity of ions from mixtures of electrolytes inside nanopores", J. Chem. Phys. 2008, 129:224703.
- Taboada-Serrano, P.; Hou, C.-H.; Vithayaveroj, V.; Yiacoumi, S., Tsouris, C. "Comparison between Effective Electrode/Eletrolyte Interface Potential and Applied Potential for Gold Electrodes", Ind. Eng. Chem. Res. 2008, 47:3525.
- Hou, C.-H.; Taboada-Serrano, P.; Yiacoumi, S.; Tsouris, C. "Monte Carlo Simulations of Electrical Double-layer Formation from Mixtures of Electrolytes inside Nanopores", J. Chem. Phys. 2008, 128:044705.
- Szymcek, P.; McCallum, S.D.; Taboada-Serrano, P.; Tsouris, C. "A Pilot-Scale Continuous-Jet Hydrate Reactor", Chem. Eng. J. 2008, 135:71.
- Tsouris, C.; Szymcek, P.; Taboada-Serrano, P.; McCallum, S.D.; Adams, E.; Chow, A.; Brewer P.; Peltzer, E.; Walz, P.; Johnson, W.K.; Summers, J. "Scaled-up Ocean Injection of CO_2-hydrate Composite Particles", Energy & Fuels 2007, 21:3300.
- Taboada-Serrano, P.; Yiacoumi, S.; Tsouris, C. "Electrostatic Surface Interactions in Mixtures of Symmetric and Asymmetric Electrolytes: A Monte Carlo Study", J. Chem. Phys. 2006, 125:054716.
- Taboada-Serrano, P.; Chin, C.-J.; Yiacoumi, S.; Tsouris, C. "Modeling Aggregation of Colloidal Particles", Curr. Opin. Colloid Interface. Sci. 2005, 10:123.
- Taboada-Serrano, P.; Yiacoumi, S.; Tsouris, C. "Behavior of Symmetric and Asymmetric Electrolytes near Discretely Charged Planar Surfaces: A Monte Carlo Study", J. Chem. Phys. 2005, 123:054703.
- Taboada-Serrano, P.; Vithayaveroj, V.; Yiacoumi, S.; Tsouris, C. "Surface Charge Heterogeneities Measured by Atomic Force Microscopy", Environ. Sci. Technol. 2005, 39:6352.