

Raúl Hernández Sánchez

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❖ Employment

- Assistant Professor, University of Pittsburgh, 2018 – present
- Columbia Nano Initiative Postdoctoral Fellow, 2016 – 2018

❖ Education

- *CNI Postdoctoral Fellow*, Department of Chemistry, Columbia University, New York, NY, 01/2016 to 05/2018. Advisor: Prof. Colin Nuckolls
- *Ph.D. in Chemistry*, Department of Chemistry, Harvard University, Cambridge, MA, 08/2010 to 05/2015. Advisor: Prof. Theodore A. Betley
- *A.M. in Chemistry*, Department of Chemistry, Harvard University, Cambridge, MA, 08/2010 to 05/2012. Advisor: Prof. Theodore A. Betley
- *B.S. in Chemistry*, Department of Chemistry, ITESM Campus Monterrey, Monterrey, Mexico, 08/2005 to 05/2010. Advisor: Prof. Jesus Valencia

❖ Awards and Honors

- 2021** NSF CAREER Award.
- 2020** ACS PRF Doctoral New Investigator Award.
- 2019** SNI Level I (National System of Researchers in México).
- 2016** Columbia Nano Initiative Postdoctoral Research Scientist Fellowship.
- 2015** Poster Prize Award 5th European Conference on Molecular Magnetism.
- 2015** Fellowship from the 5th European Conference on Molecular Magnetism.
- 2015** Featured in "Las 30 promesas" (The 30 promises) emitted by Grupo Editorial Expansion.
- 2012** ACS, Division of Inorganic Chemistry Student Travel Award.
- 2011 – 2012** CONACYT/Fundación México en Harvard Research Award.
- 2010** CONACYT/Fundación Mexico en Harvard Fellowship and Research Award, Fieser Graduate Research Award.
- 2008** Research Assistant Scholarship, Caltech.
- 2007** Summer Undergraduate Research Fellowship (SURF), Caltech.
- 2005 – 2010** Xorge A. Domínguez Scholarship, ITESM.
- 2005 – 2010** Special Chemistry Scholarship L.C.Q., ITESM.
- 2004** Honorary Mention in XV Mexican Physics Olympiad.

❖ Grant Proposals Funded

6. University of Pittsburgh, Center for Research Computing, "Tubularenes: expanding the boundaries of carbon-based nanotubes". Single PI. Amount: \$0, 900,000 SUs (computational service units). Period: 03/2021-02/2022.
5. National Science Foundation, "CAREER: Tubularenes: a novel class of conjugated molecular nanotubes". Single PI. Amount: \$679,989.00. Period: 09/2021-08/2026.
4. American Chemical Society Petroleum Research Fund Doctoral New Investigator, "Recycling hydrocarbons at polynuclear reaction sites". Single PI. Amount: \$110,000.00. Period: 09/2020-08/2022.
3. University of Pittsburgh, Pitt Momentum Funds, "Fuel recycling at copper catalysts". Single PI. Amount: \$16,000.00. Period: 03/2020-06/2021.
2. University of Pittsburgh, Center for Research Computing, "Tubularenes: redefining carbon-based nanotubes". Single PI. Amount: \$0, 1,300,000 SUs (computational units). Period: 03/2020-02/2021.

1. University of Pittsburgh, Central Research Development Fund, "Tubular[n]arenes: wire-like cylindrical organic conductors". Single PI. Amount: \$18,000.00. Period: 07/2019-06/2021.

❖ **Publications (Google scholar metrics: H-index=18; 1225 citations as of 7/13/2021)**

At Pitt

36. Mirzaei, S.; Espinoza Castro, V.; **Hernández Sánchez, R.*** "Quantum confinement at molecular carbon-based nanotubes". *In preparation*.
35. Osei, M.; Mirzaei, S.; **Hernández Sánchez, R.*** "Cuprophilic and argentophilic interactions between tetranuclear clusters". *In preparation*.
34. Osei, M.; Mirzaei, S.; Rahman, M. A.; Castro, E.; **Hernández Sánchez, R.*** "C₄-symmetric square planar tetranuclear copper clusters". *In preparation*.
33. Mirzaei, S.; Espinoza Castro, V.; **Hernández Sánchez, R.*** "Nonspherical anion recognition by supramolecular cages: towards the sequestration of PFAS". *In preparation*.
32. Mirzaei, S.; Castro, E.; **Hernández Sánchez, R.*** "Conjugated Molecular Nanotubes". *Chem. Eur. J.* **2021**, *27*, 8642.
31. Castro, E.;[§] Mirzaei, S.;[§] **Hernández Sánchez, R.*** "Radially Oriented [n]Cyclo-meta-phenylenes". *Org. Lett.* **2021**, *23*, 87. § = contributed equally.
30. Gadjeva, N. A.; Szimai, P.; Sági, O.; Alemany, P.; Conejeros, S.; Paley, D. W.; **Hernández Sánchez, R.**; Fowler, B.; Náfrádi, B.; Forró, L.; Roy, X. S.; Batail, P.>* Canadell, E.>* Steigerwald, M. L.>* Nuckolls, C.* "Intermolecular Resonance Correlates Electron Pairs Down a Supermolecular Chain: Antiferromagnetism in K-Doped p-Terphenyl". *J. Am. Chem. Soc.* **2020**, *142*, 20624.
29. Mirzaei, S.;[§] Castro, E.;[§] **Hernández Sánchez, R.*** "Tubularenes". *Chem. Sci.* **2020**, *11*, 8089. § = contributed equally.

Before Pitt

28. Liu, T.; Yang, J.; Geyer, F.; Conrad-Burton, F.; **Hernández Sánchez, R.**; Li, H.; Zhu, X.; Xiao, S.; Nuckolls, C.; Steigerwald, M. "Stringing the Perylene Diimide Bow". *Angew. Chem. Int. Ed.* **2020**, *59*, 14303.
27. Conrad-Burton, F.; Liu, T.; Geyer, F.; Costantini, R.; Schlaus, A.; Spencer, M.; Wang, J.; **Hernández Sánchez, R.**; Zhang, B.; Xu, Q.; Steigerwald, M.; Xiao, S.; Li, H.; Nuckolls, C.; Zhu, X. "Controlling Singlet Fission by Molecular Contortion". *J. Am. Chem. Soc.* **2019**, *141*, 13143.
26. Bartholomew A. K.; Teesdale, J. J.; **Hernández Sánchez, R.**; Malbrecht, B.J.; Juda, C.; Ménard, G.; Bu, W.; Iovan, D. A.; Mikhailine, A. A.; Zheng, S.-L.; Sarangi, R.; Wang, S. G.; Chen, Y.-S.; Betley, T. A. "Exposing the inadequacy of redox formalisms by resolving redox inequivalence within isovalent clusters". *Proc. Natl. Acad. Sci.* **2019**, *116*, 15836.
25. Milton, M.; Schuster, N.; Paley, D. W.; **Hernández Sánchez, R.**; Ng, F.; Steigerwald, M. L.; Nuckolls, C. "Defying Strain in the Synthesis of an Electroactive Bilayer Helicene". *Chem. Sci.* **2019**, *10*, 1029.
24. **Hernández Sánchez, R.**; Betley, T. A. "Thermally Persistent High-Spin Ground States in Octahedral Iron Clusters". *J. Am. Chem. Soc.* **2018**, *140*, 16792.
23. **Hernández Sánchez, R.***; Champsaur, A. M.; Choi, B.; Wang, S. G.; Bu, W.; Roy, X.; Chen, Y.-S.*; Steigerwald, M. L.*; Nuckolls, C.*; Paley, D. W.*. "Electron cartography in clusters". *Angew. Chem. Int. Ed.* **2018**, *57*, 13815.
22. Schuster, N.; **Hernández Sánchez, R.**; Bukharina, D.; Kotov, N. A.; Breova, N.; Ng, F.*; Steigerwald, M. L.*; Nuckolls, C.*. "A Helicene Nanoribbon with Greatly Amplified Chirality". *J. Am. Chem. Soc.* **2018**, *140*, 6235.
21. Zhang, B.;[§] **Hernández Sánchez, R.**; Zhong, Y.; Ball, M.; Terban, M. W.; Paley, D.; Billinge, S. J. L.; Ng, F.; Steigerwald, M. L.; Nuckolls, C. "Hollow Organic Capsules Assemble into Cellular Semiconductors". *Nat. Commun.* **2018**, *9*, 1957. § = equal contribution.
20. Milton, M.; Cheng, Q.; Yang, Y.*; Nuckolls, C.*; **Hernández Sánchez, R.***; Sisto, T.* "Molecular materials for Non-Aqueous Flow Batteries with High Coulombic Efficiency and Stable Cycling". *Nano Lett.* **2017**, *17*, 7859.

19. Keener, M.; Peterson, M.; **Hernández Sánchez, R.**; Oswald, V. F.; Wu, G.; Ménard, G.*. “Towards Catalytic Ammonia Oxidation to Dinitrogen: A Synthetic Cycle Using a Simple Manganese Complex”. *Chem. Eur. J.* **2017**, *23*, 11479.
18. Amiri, H.; Shepard, K.*; Nuckolls, C.*; **Hernández Sánchez, R.***. “Single-Walled Carbon Nanotubes: Mimics of Biological Ion Channels”. *Nano Lett.* **2017**, *17*, 1204.
17. Lee, H.; Campbell, M. G.; **Hernández Sánchez, R.**; Börgel, J.; Raynaud, J.; Parker, S. E.; Ritter, T. “Mechanistic Insight Into High-Spin Iron(I)-Catalyzed Butadiene Dimerization”. *Organometallics* **2016**, *35*, 2923.
16. Furneaux, A. G.; Piro, N. A.; **Hernández Sánchez, R.**; Garmigna, K. M.; Fey, N.; Robinson, M. J.; Kassel, W. S.; Nataro, C. “Spectroscopic, structural and computational analysis of $[\text{Re}(\text{CO})_3(\text{dippM})\text{Br}]^{n+}$ (dippM = 1,1'-bis(diiso-propylphosphino)metallocene, M = Fe, $n = 0$ or 1; M = Co, $n = 1$)”. *Dalton Trans.* **2016**, *45*, 4819.
15. Blass, B. L.; **Hernández Sánchez, R.**; Decker, V. A.; Robinson, M. J.; Piro, N. A.; Kassel, W. S.; Diaconescu, P. L.; Nataro, C. “Structural, Computational, and Spectroscopic Investigation of $[\text{Pd}(\kappa^3\text{-}1,1'\text{-bis}(\text{di-tert-butylphosphino})\text{ferrocenediyl})\text{X}]^+$ (X = Cl, Br, I) Compounds”. *Organometallics* **2016**, *35*, 462.
14. **Hernández Sánchez, R.**; Bartholomew, A.; Powers, T.; Ménard, G.; Betley, T. A. “Maximizing electron exchange in a $[\text{Fe}_3]$ cluster”. *J. Am. Chem. Soc.* **2016**, *138*, 2235.
13. **Hernández Sánchez, R.**; Betley, T. A. “Meta-Atom Behavior in Clusters Revealing Large Spin Ground States”. *J. Am. Chem. Soc.* **2015**, *137*, 13949.
12. **Hernández Sánchez, R.**; Zheng, S.-L.; Betley, T. A. “Ligand Field Strength Mediates Electron Delocalization in Octahedral $[(^{\text{H}}\text{L})_2\text{Fe}_6(\text{L}')_m]^{n+}$ Clusters”. *J. Am. Chem. Soc.* **2015**, *137*, 11126.
11. **Hernández Sánchez, R.**; Willis, A. M.; Zheng, S.-L.; Betley, T. A. “Synthesis of Well-Defined Bicapped Octahedral Iron Clusters $[(^{\text{ten}}\text{L})_2\text{Fe}_8(\text{PMe}_2\text{Ph})_2]^n$ ($n = 0, -1$)”. *Angew. Chem. Int. Ed.* **2015**, *54*, 12009.
10. Cramer, S. A.; **Hernández Sánchez, R.**; Brakhage, D. F.; Jenkins, D. M. “Probing the role of an Fe^{IV} tetrazene in catalytic aziridination”. *Chem. Commun.* **2014**, *50*, 13967.
9. Wu, B.; **Hernández Sánchez, R.**; Bezpalko, M. W.; Foxman, B. M.; Thomas, C. M. “Formation of a Heterobimetallic Zirconium/Cobalt Diimido Complexes via a Four-Electron Transformation”. *Inorg. Chem.* **2014**, *53*, 10021.
8. Powers, T. M.; Gu, N. X.; Fout, A. R.; Baldwin, A. M.; **Hernández Sánchez, R.**; Alfonso, D. M.; Chen, Y.-S.; Zheng, S.-L.; Betley, T. A. “Synthesis of Open-Shell, Bimetallic Mn/Fe Trinuclear Clusters”. *J. Am. Chem. Soc.* **2013**, *135*, 14448.
7. Eames, E.; **Hernández Sánchez, R.**; Betley, T. A. “Metal atom lability in polynuclear complexes”. *Inorg. Chem.* **2013**, *56*, 5006.
6. Kraft, S. J.; **Hernández Sánchez, R.**; Hock, A. S. “A Remarkably Active Iron Catecholate Immobilized in a Porous Organic Polymer”. *ACS Catal.* **2013**, *3*, 826.
5. Wong, L. J.; **Hernández Sánchez, R.**; Glancy Logan, J.; Zarkesh, R. A.; Ziller, J. W.; Heyduk, A. F. “Disulfide reductive elimination from an iron(III) complex”. *Chem. Sci.* **2013**, *4*, 1906.
4. Harris, T. D.; Zhao, Q.; **Hernández Sánchez, R.**; Betley, T. A. “Expanded Redox Accessibility via Ligand Substitution in an Octahedral Fe_6Br_6 Cluster”. *Chem. Commun.* **2011**, *47*, 6344.
3. Yamazaki, Y.; **Hernandez-Sanchez, R.**; Haile, S. M. “Cation nonstoichiometry in yttrium-doped barium zirconate: phase behavior, microstructure, and proton conductivity”. *J. Mater. Chem.* **2010**, *20*, 8158-8166.
2. Telila, H.; Mamo, T.; **Hernandez Sanchez, R.** “The Fabrication of nanoparticle CsH_2PO_4 Electrolyte for Fuel Cell Applications”. *Caltech Undergraduate Research Journal* **2009**, Vol. 9 (No. 1), 33 – 39.
1. Yamazaki, Y.; **Hernandez-Sanchez, R.**; Haile, S. M. “High Total Proton Conductivity in Large-Grained Yttrium-Doped Barium Zirconate”. *Chem. Mater.* **2009**, *21* (13), 2755-2762.

❖ Patents

2. Mirzaei, S.; Castro, E.; Hernández Sánchez, R. “Synthesis of Nanotubular Molecules”. U.S. Provisional Patent **US 63/057,506** filed July 28th, 2020.
1. Milton, M.; Cheng, Q.; Yang, Y.*; Nuckolls, C.*; **Hernández Sánchez, R.***; Sisto, T.* “Non-Aqueous Flow Batteries”. **US 16/792,501** and **WO 2019/036633 A1**.

❖ Synergistic Activities and Contributions to Diversity

4. Faculty support for the Alliance for Diversity in Science and Engineering (ADSE) Chapter at the University of Pittsburgh. **2019 – present**.
3. Mentor at Eureka Street Corporation (www.eurekastreet.org). **2018 – present**. Student mentoring program to support students from minority serving institutions on their applications to graduate programs in Physics and Chemistry in the USA. Students mentored (2018-present) = 3.
2. City Coordinator of “Clubes de Ciencia México” (www.clubesdeciencia.mx). **2017 – present**. Science outreach program designed to bring hands-on week-long workshops in STEM to high school and undergraduate students in Mexico. The instructors are PhD/postdocs volunteers from top universities in the United States and Mexico.
1. PQI Quantum Day, **April 2019**. Science outreach to show high school students the day-to-day work of a researcher through a laboratory tour.

❖ Collaborators

Collaborators at the University of Pittsburgh: Professor James McKone and Professor Göetz Vesper (Department of Chemical and Petroleum Engineering).

Collaborators at Argonne National Laboratory: Dr. Yu-Sheng Chen (ChemMatCARS – The University of Chicago).

Collaborators at Georgia Institute of Technology: Dr. Juan Pablo Correa-Baena (School of Materials Science and Engineering).

Collaborators at Université Paris-Saclay, Orsay: Dr. Pawel Wzietek (Laboratoire de Physique des Solides).

Collaborators at University of Angers (CNRS): Dr. Patrick Batail.

Graduate Advisor: Professor Theodore A. Betley (Harvard).

Postdoctoral Sponsors: Professor Colin Nuckolls (Columbia) and Columbia Nano Initiative.

❖ Mentorship

Current: Ph.D. students: (7) Swati Arora, Victor Espinoza Castro, Saber Mirzaei, Keren Lee, Brett Lucht, Manasseh Osei, and Mohammad Azizur Rahman.

Past: postdoctoral supervision: (2) Dr. Thomas Allen and Dr. Edison Arley Castro Portillo.

Undergraduate students: (8) Nicolas D'Annunzio, Ryan W. McLane, Madison Keating, James Dages, Bridget Glessner, Addison Averill, Derek Lamb, and Emily Nicola.

❖ Teaching Accomplishments

- Chemistry 1130/Chemistry 2180, Spring 2021 – Inorganic Chemistry (capstone course) – 2 graduate and 26 undergraduate students.
- Chemistry 2120, Fall 2020 – Descriptive Inorganic and Organometallic Chemistry – 17 PhD students.
- Chemistry 1130, Spring 2020 – Inorganic Chemistry (capstone course) – 33 undergraduate students.
- Chemistry 2120, Fall 2019 – Descriptive Inorganic and Organometallic Chemistry – 17 PhD students.
- Chemistry 2120, Fall 2018 – Descriptive Inorganic and Organometallic Chemistry – 18 PhD students.

❖ Invited Presentations

27. Breaking Barriers Through Chemistry, International Conference (online), August **2021**.
26. The College of New Jersey, departmental seminar (online), March **2021**.

25. American Chemical Society, Division of Inorg. Chem., National Conference (online), Feb **2021**.
24. Autonomous University of Juarez City, October **2020**, Juarez City (online), Mexico.
23. Tesla Institute, June **2020**, Juarez City (online), México.
22. Hampton University, October **2019**, Hampton, VA, USA.
21. University of Maryland, October **2019**, College Park, MD, USA.
20. Northwestern University, September **2019**, Evanston, IL, USA.
19. University of Colorado Boulder, February **2018**, Boulder, CO, USA.
18. Indiana University Bloomington, February **2018**, Bloomington, IN, USA.
17. University of California San Diego, January **2018**, San Diego, CA, USA.
16. University of California Riverside, January **2018**, Riverside, CA, USA.
15. University of Pittsburgh, January **2018**, Pittsburgh, PA, USA.
14. University of Illinois Urbana-Champaign, January **2018**, Champaign, IL, USA.
13. Princeton University, January **2018**, Princeton, NJ, USA.
12. University of Minnesota, December **2017**, Minneapolis, MN, USA.
11. Tufts University, December **2017**, Medford, MA, USA.
10. Duke University, December **2017**, Durham, NC, USA.
9. University of Massachusetts Amherst, December **2017**, Amherst, MA, USA.
8. Columbia Friday Synthesis Symposium, November **2017**, New York, USA.
7. Boston Regional Inorganic Colloquium (BRIC, Harvard), April **2017**, Cambridge, MA.
6. MRSEC Seminar, Columbia University, October **2016**, New York, USA.
5. Nanostructure in the City Symposium, October **2016**, New York, USA.
4. Columbia Friday Synthesis Symposium, May **2016**, New York, USA.
3. Undergraduate Chemistry Seminar (ITESM), October **2015**, Monterrey, México.
2. MIT Enterprise Forum Mexico, August **2015**, Oaxaca, México.
1. Movimiento NOMADX, August **2015**, Chihuahua, México.

❖ **Contributed Presentations**

17. American Chemical Society National Meeting, August **2019**, San Diego, CA.
16. MRSEC retreat seminar, Columbia University, May **2017**, New York, USA.
15. American Chemical Society National Meeting, April **2017**, San Francisco, CA.
14. Gordon Research Conference and Seminar: Inorg. Reaction Mech., March **2017**, Houston, TX.
13. 5th European Conference on Molecular Magnetism, September **2015**, Zaragoza, Spain.
12. American Chemical Society National Meeting, August **2015**, Boston, MA.
11. American Chemical Society National Meeting, August **2014**, San Francisco, CA.
10. Gordon Research Conference and Seminar: Inorganic Chemistry, June **2014**, Biddeford, MA.
9. American Chemical Society National Meeting, April **2013**, New Orleans, LA.
8. American Chemical Society National Meeting, March **2012**, San Diego, CA.
7. Boston Regional Inorganic Colloquium (BRIC), October **2011**, Worcester, MA.
6. Bachelor Thesis Proposal Seminar, November **2009**, Monterrey, México.
5. Undergraduate Chemistry Seminar: “Nanodics at interfaces: combined application of SPR and AFM”, October **2009**, Monterrey, México.
4. Undergraduate Chemistry Seminar: “Yttrium-Doped Barium Zirconate. Defect Chemistry Study to Understand its Protonic Conductivity”, November **2008**, Monterrey, México.
3. Undergraduate Chemistry Seminar: “Effect of Barium Deficiency on the Proton Conductivity of $Ba_{1-x}Zr_{0.8}Y_{0.2}O_{3-\delta}$ ”, September **2007**, Monterrey, México.
2. Summer Undergraduate Research Fellowship Seminar: “Effect of Barium Deficiency on the Proton Conductivity of $Ba_{1-x}Zr_{0.8}Y_{0.2}O_{3-\delta}$ ”, August **2007**, Pasadena, CA.
1. Undergraduate Chemistry Seminar: “Thermal Differential Analysis of a Vitreous Sample”, November **2006**, Monterrey, México.