

## **Raúl Hernández Sánchez**

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### ❖ **Employment**

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

### ❖ **Education**

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- *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**

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- 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**

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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; 1259 citations as of 8/29/2021)**

*At Pitt (independent career, \* = corresponding author)*

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. Mirzaei, S.; Espinoza Castro, V.; **Hernández Sánchez, R.\*** "Nonspherical anion recognition by supramolecular cages". *Submitted*.
33. Osei, M.; Mirzaei, S.; Rahman, M. A.; Castro, E.; **Hernández Sánchez, R.\*** "Hole delocalization within square planar [Cu<sub>4</sub>] clusters". *Submitted*.
32. Mirzaei, S.; Castro, E.; **Hernández Sánchez, R.\*** "Conjugated Molecular Nanotubes". *Chem. Eur. J.* **2021**, *27*, 8642.
31. Castro, E.;<sup>§</sup> Mirzaei, S.;<sup>§</sup> **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.;<sup>§</sup> Castro, E.;<sup>§</sup> **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.;<sup>§</sup> **Hernández Sánchez, R.**;<sup>§</sup> 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 Biccapped 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  $\text{Fe}^{\text{IV}}$  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  $\text{Fe}_6\text{Br}_6$  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  $\text{CsH}_2\text{PO}_4$  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

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### *At Pitt (independent career)*

2. Mirzaei, S.; Castro, E.; Hernández Sánchez, R. “Synthesis of Nanotubular Molecules”. U.S. Non-Provisional Patent **US 17/386,100** filed July 27<sup>th</sup>, 2021.

### *As postdoc*

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**.

## ❖ Books

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### *At Pitt (independent career)*

1. Castro, E.; Mirzaei, S.; **Hernández Sánchez, R.\*** “Carbon-based nanotubes”. De Gruyter, *in editorial production*.

## ❖ Synergistic Activities and Contributions to Diversity

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4. Founder of Tips For Students (TFS), designed to guide undergraduates in their career decision making process by conveying the story of recent bachelor graduates working in academia and industry. **June 2021 – present**.
3. Faculty support and founder of the Alliance for Diversity in Science and Engineering (ADSE) Chapter at the University of Pittsburgh. **2019 – present**. Last activity in Feb 2021 gathered ~700 high school students in Pittsburgh.
2. Mentor at Eureka Street Corporation ([www.eurekastreet.org](http://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.
1. City Coordinator of “Clubes de Ciencia México” ([www.clubesdeciencia.mx](http://www.clubesdeciencia.mx)). **2017 – present**. Science outreach program designed to bring hands-on week-long workshops in STEM to students in high school and undergraduate in Mexico. The instructors are PhD/postdocs volunteers from top universities in the United States and Mexico. Since my involvement, we have reached more than 500 students in Chihuahua City.

## ❖ Collaborators

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*Collaborators at University of Pittsburgh:* Prof. Sunil Saxena, Prof. Peng Liu, Prof. James Mckone, and Prof. Nathaniel Rosi (Department of Chemistry).

*Collaborators at University of Texas, El Paso:* Prof. Luis Echegoyen (Department of Chemistry and Biochemistry).

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

*Collaborators at Georgia Institute of Technology:* Prof. 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):* Prof. Patrick Batail.

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

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

## ❖ Mentorship

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*Current: Ph.D. students:* (5) Swati Arora, Victor Espinoza Castro, Brett Lucht, Saber Mirzaei, and Manasseh Osei.

*Past: postdoctoral supervision:* (2) Dr. Edison Arley Castro Portillo, Dr. Thomas Allen. *Undergraduate students:* (8) Nicolas D'Annunzio, Ryan W. McLane, Madison Keating, James Dages, Bridget Glessner, Addison Averill, Derek Lamb, and Emily Nicola.

#### ❖ Teaching Accomplishments

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- Chemistry 2120, Fall 2021 – Descriptive Inorganic and Organometallic Chemistry – 16 PhD students.
- 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

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27. Breaking Barriers Through Chemistry, sponsored by Thieme and The University of Texas A&M (online), August **2021**.
26. The College of New Jersey, departmental seminar (online), March **2021**.
25. American Chemical Society, Division of Inorganic Chemistry “Periodic Table Talks”, 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

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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  $\text{Ba}_{1-x}\text{Zr}_{0.8}\text{Y}_{0.2}\text{O}_{3-\delta}$ ”, September **2007**, Monterrey, México.
2. Summer Undergraduate Research Fellowship Seminar: “Effect of Barium Deficiency on the Proton Conductivity of  $\text{Ba}_{1-x}\text{Zr}_{0.8}\text{Y}_{0.2}\text{O}_{3-\delta}$ ”, August **2007**, Pasadena, CA.
1. Undergraduate Chemistry Seminar: “Thermal Differential Analysis of a Vitreous Sample”, November **2006**, Monterrey, México.