

Raúl Hernández Sánchez

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❖ Employment

- Norman Hackerman Welch Young Investigator, Assistant Professor, Rice University, 2022 – present
- Adjunct Professor, University of Pittsburgh, 2022 – present
- Assistant Professor, University of Pittsburgh, 2018 – 2022
- 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

9. NSF MRI, "MRI: Acquisition of a Single Crystal X-Ray Diffractometer for Research and Education with Regional Impact". Collaborative. Amount: \$308,651.70. Period: 9/2022-8/2025.
Note: this grant was transferred to co-PI Prof. Nathaniel Rosi due to departure to Rice University.
8. National Science Foundation, "ERASE-PFAS: Bottom-up synthesis of polymeric membranes for PFAS sequestration". Single PI. Amount: \$419,999.00. Period: 10/2022-08/2025.
7. Royal Society of Chemistry, Inclusion & Diversity Fund, "Science Clubs Mexico 2022: Inclusion and Diversity in Chemistry Education". Collaborative. Amount: £5,000.00. Period: 01/2022-08/2022.
6. University of Pittsburgh, Center for Research Computing, "Tubularenes: expanding the boundaries of carbon-based nanotubes". Single PI. Amount: \$0, 900,000 SUs per year (computational service units). Period: 03/2021-02/2023.
5. National Science Foundation, "CAREER: Tubularenes: a novel class of conjugated molecular nanotubes". Single PI. Amount: \$598,844.00. Period: 11/2022-12/2026.

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=20; 1638 citations as of 1/22/2023)**

Independent career (*=corresponding author; §=equal contribution; undergraduate authors underlined)

40. Mirzaei, S.; Hernández Sánchez, R.* "Green emitting molecular nanotube". *In preparation*.
39. Arora, S.; Mirzaei, S.; Espinoza Castro, V.; Hernández Sánchez, R.* "Removal of PFAS from water at environmentally-relevant concentrations". *In preparation*.
38. Mirzaei, S.; Hernández Sánchez, R.* "Catching fullerenes: synthesis of a molecular nanoglove". *In preparation*.
37. Mirzaei, S.; Espinoza Castro, V.; Prieto, Gabriella; Hernández Sánchez, R.* "Quantum confinement at molecular nanotubes". *In preparation*.
36. Osei, M.; Mirzaei, S.; Hernández Sánchez, R.* "Reversible dioxygen uptake at [Cu₄] clusters ". *In preparation*.
35. Osei, M.; Mirzaei, S.; Hernández Sánchez, R.* "Metallophilic interactions in square planar coinage clusters". *In preparation*.
34. Osei, M.; Mirzaei, S.; Bogetti, X.; Rahman, M. A.; Castro, E.; Saxena, S.; Hernández Sánchez, R.* "Synthesis of square planar Cu₄ clusters ". *Angew. Chem. Int. Ed.* **2022**, *61*, 41, e202209529.
33. Mirzaei, S.; Espinoza Castro, V.; Hernández Sánchez, R.* "Nonspherical anion sequestration by C-H hydrogen bonding". *Chem Sci.* **2022**, *13*, 2026.
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.
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.

PhD and postdoc

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.
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 $[\text{Pd}(\kappa^3\text{-}1,1'\text{-bis}(\text{di-}t\text{-}ert\text{-}butylphosphino)ferrocenediyl)\text{X}]^+$ (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 $[(^H\text{L})_2\text{Fe}_6(\text{L}')_m]^{n+}$ 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 $[(^{\text{trent}}\text{L})_2\text{Fe}_8(\text{PMe}_2\text{Ph})_2]^n$ ($n = 0, -1$)”. *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 Fe₆Br₆ 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 CsH₂PO₄ 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

Independent career

3. Arora, S.; Mirzaei, S.; Espinoza Castro, V. M.; Hernández Sánchez, R. “Compositions comprising macrocyclic hosting moieties”. U.S. Provisional Patent **63/302,923**.
2. Mirzaei, S.; Castro, E.; Hernández Sánchez, R. “Synthesis of Nanotubular Molecules”. U.S. Non-Provisional Patent **US 17/386,100** filed July 27th, 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

Independent career

1. Castro, E.; Mirzaei, S.; **Hernández Sánchez, R.*** “Carbon-based nanotubes”. De Gruyter, *published April 2022*.

❖ Invited Presentations

Independent career. **2023:** University of California, Irvine (April). **2022:** Supramolecular and Organic Materials Chemistry ACS SWRM (Nov), Gulf Coast Undergraduate Research Symposium (Oct, keynote speaker), University of Central Florida (Sept), Young Research Conference ADSE (May), Rice University (Feb), University of Houston (Feb). **2021:** Breaking Barriers Through Chemistry sponsored by Thieme (Aug), The College of New Jersey (March), ADC DIC “Periodic Table Talks” (Feb), Autonomous University of Juarez City (Oct). **2020:** Tesla Institute (June). **2019:** Hampton University (Oct), University of Maryland (Oct), Northwestern University (Sept). PhD and Postdoc. **2018:** University of Colorado Boulder (Feb), Indiana University Bloomington (Feb), University of California San Diego (Jan), University of California Riverside (Jan), University of Pittsburgh (Jan), University of Illinois Urbana-Champaign (Jan), Princeton University (Jan). **2017:** University of Minnesota (Dec), Tufts University (Dec), Duke University (Dec), University of Massachusetts Amherst (Dec), Columbia Friday Synthesis Symposium (Nov), Boston Regional Inorganic Colloquium (April). **2016:** MRSEC Seminar Columbia University (Oct), Nanostructure in the City Symposium (Oct), Columbia Friday Synthesis Symposium (May). **2015:** Undergraduate Chemistry Seminar at ITESM (Oct), MIT Enterprise Forum Mexico (Aug), Movimiento NOMADX (Aug).

❖ Contributed Presentations

Independent career. **2023:** GRC Inorganic Reaction Mechanisms (Mar). **2022:** 16th International Symposium on Macrocyclic and Supramolecular Chemistry (June). **2022:** ACS National Meeting (Mar). **2019:** ACS National Meeting (Aug). PhD and Postdoc. **2017:** MRSEC retreat seminar at Columbia University (May), ACS National Meeting (April), GRC Inorganic Reaction Mechanisms (Mar). **2015:** 5th European Conference on Molecular Magnetism (Sept), ACS National Meeting (Aug). **2014:** ACS National Meeting (Aug), GRC and GRS Inorganic Chemistry (June). **2013:** ACS National Meeting (April). **2012:** ACS National Meeting (Mar). **2011:** Boston Regional Inorganic Colloquium (Oct). **2009:** Bachelor Thesis Proposal Seminar (Nov), Undergraduate Chemistry Seminar at ITESM (Oct). **2008:** Undergraduate Chemistry Seminar at ITESM (Nov). **2007:** Undergraduate Chemistry Seminar at ITESM (Sept), SURF Seminar at Caltech (Aug). **2006:** Undergraduate Chemistry Seminar at ITESM (Nov).