

# Jose L. Mendoza-Cortes

## Assistant Professor

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## Appointments

Institution	Department/Program	Location	Position	Year
Florida State University	Chem. and Biomedical Eng.	Tallahassee, FL	Assistant Prof.	2015 -
Florida A&M University	Chem. and Biomedical Eng.	Tallahassee, FL	Assistant Prof.	2015 -
Florida State University	High Performance Mat. Inst.	Tallahassee, FL	Assistant Prof.	2015 -
Florida State University	Scientific Computing	Tallahassee, FL	Affiliated Faculty	2015 -
Florida State University	Materials Science and Eng.	Tallahassee, FL	Affiliated Faculty	2015 -
Nat'l High Magnetic Lab	Condensed Matter Science	Tallahassee, FL	Scientist	2015 -

## Education

Institution	Major/Area	Location	Degree	Year
UC Berkeley/ Berkeley National Lab	Theoretical Chemistry	Berkeley, CA	Postdoc	2014
California Institute of Technology	Solid State Physics	Pasadena, CA	Staff Sci.	2013
Joint Center for Artificial Photosynthesis	Applied Physics	Pasadena, CA	Staff Sci.	2013
California Institute of Technology	Condense Matter Sci.	Pasadena, CA	Postdoc	2013
California Institute of Technology	Materials Science	Pasadena, CA	Ph.D.	2012
California Institute of Technology	Materials Science	Pasadena, CA	M.Sc.	2010
Tec de Monterrey (ITESM)	Physical Chemistry	Monterrey, NL	B.Sc.	2008
University of California, Los Angeles	Materials Chemistry	Los Angeles, CA		2006

## Scientific pedigree

*PhD* | J.L. Mendoza-Cortes obtained his Ph.D. in 2012 from William Godddard III at Caltech in USA.  
William Godddard III obtained his Ph.D. in 1964 from Pol Duwez at Caltech in USA.  
Pol Duwez received his D.Sc. in 1933 from Emile Henriot at U. Brussels in Belgium.  
Emile Henriot received his D.Sc. in 1912 from *Marie Curie* at the Sorbonne in France.

*PDF* | J.L. Mendoza-Cortes did his PDF in 2014 with Martin Head-Gordon at Berkeley in USA.  
Martin Head-Gordon obtained his Ph.D. in 1989 from John Pople at Carnegie Mellon in USA.  
John Pople received his D.Sc. in 1951 from John Lennard-Jones at Cambridge in England.  
John Lennard-Jones received his D.Sc. in 1924 from Ralph H. Fowler at Cambridge in England.  
Ralph H. Fowler gave his D.Sc. in 1926 to *Paul Dirac* at Cambridge in England.

## Research Articles

**Citations: 3690**, Source: Google Scholar

\* = Corresponding Author. ‡ = Authors contributed equally.

1. Srimanta Pakhira, Kevin P. Lucht, J. L. Mendoza-Cortes\* "Iron Intercalation in Covalent-Organic Frameworks: A Promising Approach for Semiconductors" *Journal of Physical Chemistry C*, 2017, 121 (39), 21160-21170.
2. Y. Lei, S. Pakhira, K. Fujisawa, X. Wang, O. O. Iyiola, N. P. Lopez, A. L. Elias, L. P. Rajukumar, C. Zhou, B. Kabius, N. Alem, M. Endo, R. Lv\*, J. L. Mendoza-Cortes\*, M. Terrones\*, "Low temperature synthesis of heterostructures of transition metal dichalcogenide alloys ( $W_xMo_{1-x}S_2$ ) and graphene with superior catalytic performance for hydrogen evolution" *ACS Nano*, 2017, 11, 5103-5112 .

3. Yohanes Pramudya, J. L. Mendoza-Cortes\*, “Design Principles for High H<sub>2</sub> Storage Using Chelation of Abundant Transition Metals in Covalent Organic Frameworks for 0-700 bar at 298K” *Journal of the American Chemical Society*, 2016, 138, 15204-15213.
4. Kevin P Lucht, J. L. Mendoza-Cortes\*, “Birnessite: A Layered Manganese Oxide To Capture Sunlight for Water-Splitting Catalysis” *Journal of Physical Chemistry C*, 2015, 22838-22846.
5. J. L. Mendoza-Cortes<sup>‡</sup>, M. Zhang<sup>‡</sup>, M. El-Roz<sup>‡</sup>, D. Lacy, J. C. Peters, H. Frei, Martin Head-Gordon, “Visible Light Sensitized CO<sub>2</sub> Activation by the Tetraaza [CoIIIn<sub>4</sub>H(MeCN)]<sup>2+</sup> Complex” *Journal of Physical Chemistry C*, 2015, 4645-4654.
6. J. L. Mendoza-Cortes<sup>‡</sup>, Q. An<sup>‡</sup>, W. A. Goddard, S. Zybin, “Prediction of the crystal packing of di-tetrazine-tetroxide (DTTO) energetic material” *Journal of Computational Chemistry*, 2015, 1-5.
7. J. L. Mendoza-Cortes<sup>‡</sup>, N. Nair<sup>‡</sup>, R. Abrol, W. A. Goddard III, V. Prakash Reddy, “1,3-Sigmatropic fluorine migration to boron in McLafferty type of rearrangements”, *Journal of Organometallic Chemistry*, 2013, 133-139.
8. J. L. Mendoza-Cortes<sup>‡</sup>, J. S. Kanady<sup>‡</sup>, E. Y. Tsui, W. A. Goddard and T. Agapie, “Oxygen Atom Transfer and Oxidative Water Incorporation in Cuboidal Mn<sub>3</sub>MO<sub>n</sub> Complexes based on Synthetic, Isotopic Labeling, and Computational Studies” *Journal of the American Chemical Society*, 2013, 1073-1082. <sup>‡</sup>These authors contributed equally.
9. J. L. Mendoza-Cortes, W. A. Goddard, H. Furukawa and O. M. Yaghi, “A Covalent Organic Framework that Exceeds the DOE 2015 Volumetric Target for H<sub>2</sub> Uptake at 298 K” *Journal of Physical Chemistry Letters*, 2012, 2671-2675.
10. J. L. Mendoza-Cortes, S. S. Han and W. A. Goddard, “High H<sub>2</sub> Uptake in pure, Li-, Na-, K-metalated Covalent Organic Frameworks and Metal Organic Frameworks at 298 K” *Journal of Physical Chemistry A*, 2012, 1621-1631.
11. J. L. Mendoza-Cortes, Tod A. Pascal and W. A. Goddard, “Design of Covalent Organic Frameworks for Methane Storage” *Journal of Physical Chemistry A*, 2011, 13852-13857.
12. J. L. Mendoza-Cortes, S. S. Han, H. Furukawa, O. M. Yaghi and W. A. Goddard, “Adsorption Mechanism and Uptake of Methane in Covalent Organic Frameworks: Theory and Experiment” *Journal of Physical Chemistry A*, 2010, 10824-10833.
13. S. S. Han<sup>‡</sup>, J. L. Mendoza-Cortes<sup>‡</sup> and W. A. Goddard, “Recent advances<sup>‡</sup> on simulation and theory of hydrogen storage in metal-organic frameworks and covalent organic frameworks” *Chemical Society Reviews*, 2009, 1460-1476.
14. D. J. Tranchemontagne<sup>‡</sup>, J. L. Mendoza-Cortes<sup>‡</sup>, M. O’Keeffe and O. M. Yaghi, “Secondary building units, nets and bonding in the chemistry of metal-organic frameworks” *Chemical Society Reviews*, 2009, 1257-1283.
15. H. M. El-Kaderi<sup>‡</sup>, J. R. Hunt<sup>‡</sup>, J. L. Mendoza-Cortes<sup>‡</sup>, A. P. Cote, R. E. Taylor, M. O’Keeffe and O. M. Yaghi, “Designed synthesis of 3D covalent organic frameworks” *Science*, 2007, 268-272.
16. W. Zhang, S. M. Brombosz, J. L. Mendoza and J. S. Moore, “A high-yield, one-step synthesis of o-phenylene ethynylene cyclic trimer via precipitation-driven alkyne metathesis” *Journal of Organic Chemistry*, 2005, 10198-10201.

## Book Chapters and Thesis

1. J. S. Kanady<sup>‡</sup>, J. L. Mendoza-Cortes<sup>‡</sup>, W. A. Goddard and T. Agapie, “The Oxygen-Evolving Complex of Photosystem II: Insights from Computation and Synthetic Models” *Metalloproteins: Theory, Calculations, and Experiments*, CRC Press, 2015, 165-204. <sup>‡</sup>These authors contributed equally.
2. J. L. Mendoza-Cortes, “Design of molecules and materials for applications in clean energy, catalysis and

molecular machines through quantum mechanics, molecular dynamics and Monte Carlo simulations”, *Ph.D. Thesis*, California Institute of Technology, 2012.

3. J. L. Mendoza-Cortes, “Ab initio based grand canonical Monte-Carlo simulations of CH<sub>4</sub> uptake in covalent-organic frameworks (COFs)”, *B.Sc. Thesis*, ITESM-UCLA-Caltech, 2008.

## Recent Submissions and Preprints

1. Srimanta Pakhira, Kevin P. Lucht, J. L. Mendoza-Cortes\* “An Alternative Strategy to Control the Electronic Properties of Bilayer Graphene: Semi-metal to Metal Transition and a Rare 2D Material with Dirac Cone”  
Preprint: arXiv:1610.04777
2. Alexander A. Aduenko, Andy Murray J. L. Mendoza-Cortes\* “Generalization of the adsorption process in crystalline porous materials and its application to Metal-Organic Frameworks (MOFs)”  
Preprint: arXiv:1401.2630
3. Ricardo Pablo-Pedro, Hector Lopez-Rios, J. L. Mendoza-Cortes, Jing Kong, Serguei Fomine, Troy Van Voorhis, Mildred S. Dresselhaus “Exploring Low Internal Reorganization Energies for Silicene Nanoclusters”  
Preprint: arXiv:1708.05369

## Selected Conference Proceedings

1. J. L. Mendoza-Cortes, Martin Head-Gordon, “Selective electrocatalytic reduction of CO<sub>2</sub> to CO in the presence of proton and water using a Co based molecular catalyst: A theoretical study of the reaction mechanism” *Abstracts of Papers of the American Chemical Society*, 2014, 248-PHYS.
2. J. L. Mendoza-Cortes, Nahid P Khiabani, William A Goddard III, “Molecular dynamics studies on the Electrical Double layer at the liquid/electrode interface” *Abstracts of Papers of the American Chemical Society*, 2014, 498-COMP.
3. J. L. Mendoza-Cortes, Yubo Su, William A Goddard III, “Transferrable force fields for van der Waals interactions” *Abstracts of Papers of the American Chemical Society*, 2014, 401-COMP.
4. J. L. Mendoza-Cortes, William A Goddard III, Hiroyasu Furukawa, Omar Yaghi, “Design principles to exceed the DOE 2017 standards for delivery and storage of H<sub>2</sub> at room temperature using nitrogen bases covalent organic frameworks” *Abstracts of Papers of the American Chemical Society*, 2014, 599-ENFL.
5. J. L. Mendoza, H. M. El-Kaderi, J. R. Hunt, A. P. Cote and O. M. Yaghi, “Covalent Organic Frameworks” *Abstracts of Papers of the American Chemical Society*, 2007, 438-ORG.
6. H. Furukawa, H. El-Kaderi, K.S. Park, J.R. Hunt, J. L. Mendoza-Cortes, A. P. Cote and O. M. Yaghi, “Metal-organic and covalent organic frameworks (MOFs and COFs) as adsorbents for environmentally significant gases (H<sub>2</sub>, CO<sub>2</sub>, and CH<sub>4</sub>)” *Abstracts of Papers of the American Chemical Society*, 2007, 291-PHYS.

## Funding Record

Involvement in Funding ~ 1 Million

PI = Project Leader. Co-PI = Project Co-Leader. FP = Faculty Participant.

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|------|---|
| 2017 | FP. National Science Foundation (NSF) - Research Experiences for Undergraduates. NSF-REU site: Sunshine Institute for the Interaction of Light with Matter. \$315,000 |
| 2016 | Co-PI. National Science Foundation (NSF). Investigation of new materials for lithium batteries and the fundamental understanding of their cycling. \$510,000          |

- 2016 PI. PG award. Understanding Cement using ab initio atomistic simulations towards smart concrete and sustainable cement. \$12,996.00
- 2016 PI. NVIDIA. Donation of 3,000 GPUs for double precision computing, a worth of \$7,000.
- 2016 PI. National Energy Research Scientific Computing Center (NERSC), Office of Science of the U.S. Department of Energy (DOE). Development of Multiscale Methods. 2016-2017. 50,000 MPP hours
- 2016 PI. First Year Assistant Professor Award. Florida State University. 2016-2017. \$20,000
- 2009 PhD Fellowship. Roberto Rocca Fellowship. 2009-2011. \$40,000.
- 2009 Conference Travel Grant. Graduate Student Office, California Institute of Technology. \$2,127.
- 2006 Mexican Ministry of Education (SEP). Young Investigator Award-Fellowship. \$50,000 MXN.
- 2005 Snyder Research Scholarship. UI at Urbana-Champaign. \$3,900.
- 2005 Xorge A. Dominguez Chemistry Award. ITESM. 2005-2008. \$36,000 MXN.
- 2003 National Council of Science and Technology Fellowship. CONACYT. 2003-2008. \$60,000 MXN.

## Selected Invited Talks

- 2016/12 “Computational materials method for clean, sustainable and cheap energy”, Oak Ridge National Laboratory, Materials Theory Group. Oak Ridge, TN. 12/2016.
- 2016/09 “Solid State Chemistry and their application to discovery of new materials”, International Mexican Congress of Chemistry, Pachuca, Mexico.
- 2016/08 “New Computational Methods and Their Applications to Producing and Storing Clean and Sustainable Energy”, Workshop on Collective Phenomena in Layered and 2D Materials, Oak Ridge, TN.
- 2016/05 “Water splitting and sunlight capture using discovery by computational methods”, The Florida Section of the American Chemical Society, Tampa, FL.
- 2016/05 “Application of new multiscale simulations for crystalline polymer and porous materials”, The Florida Section of the American Chemical Society, Tampa, FL.
- 2016/03 “New Computational Methods and its Applications to Clean and Sustainable Energy: Towards the Carbon Neutral Holy Grail”, University of Central Florida, Orlando, FL.
- 2016/02 “Sustainable Energy by Computation, Center for Research and Advanced Studies of the National Polytechnic Institute (CINVESTAV-IPN), Mexico City, Mexico.
- 2016/02 “New Computational methods and its applications to a carbon Neutral Source of Energy”, El Colegio de Mexico, Mexico City, Mexico.
- 2015/07 “Packing of Molecular Crystals”, Chemistry and Biochemistry Department, Materials Program, Florida State University, Tallahassee, FL, USA.
- 2015/07 “Theoretical Methods for Renewable Energy”, Condensed Matter Theory, National High Magnetic Field Laboratory (MagLab), Tallahassee, FL, USA.
- 2014/03 “Simulations & Computational engineering and their application to energy and materials”, Chemical and Biomedical Engineering, Florida State University, Tallahassee, FL, USA.
- 2014/01 “Generation, Transformation and Storage of Chemical Energy”, Department of Chemistry and Biochemistry, University of California Los Angeles, Los Angeles, CA, USA.
- 2013/11 “Artificial Photosynthesis; a path to alternative energy”, 3rd annual Latino students (AYM) conference, Pasadena Youth Center and Pasadena City College, Pasadena, CA, USA.
- 2013/10 “Large scale ab initio calculations for excited states and light conversion”, Special Seminar on photoexcited systems, Dept. of Chemistry, Harvard University, Cambridge, MA, USA.

- 2013/01 | “A first principles approach to energy storage and conversion”, Department of Chemistry, University of Minnesota - Twin cities, Minneapolis, MN, USA.
- 2013/03 | “Production and Storage of Renewable Clean Energy from First Principles”, Dept. of Material Sciences and Mechanical Eng., University of Maryland, College Park, MD, USA.

## Selected Honors and Awards

- 2017 | ONR Faculty Summer Fellowship. Washington D.C., USA.
- 2016 | CRC First Year Assistant Professor Award, Florida.
- 2009 | Roberto Rocca Graduate Fellowship, 15 fellows per year worldwide. Buenos Aires, Argentina.
- 2009 | ICMR fellowship, 13 fellows per year worldwide. UCSB, Santa Barbara, CA, USA. Declined.
- 2007 | AAAS Newcomb Cleveland Prize, best paper of the year in *Science* magazine. The American Association for the Advancement of Science (AAAS)’s oldest award. For the metal-free organic frameworks achieves what one reviewer described as a “holy grail” in organic materials chemistry. Boston, MA, USA
- 2007 | Glenn T. Seaborg Symposium - Poster award. Dept. Chem&Biochem, UCLA, CA, USA
- 2006 | Young scientist award, Mexican Ministry of Education (SEP). Mexico City, Mexico.
- 2005 | Snyder Research Fellowship, University of Illinois at Urbana-Champaign. Urbana, IL, USA.
- 2004 | Xorge A. Dominguez Fellowship, 20 fellows nationwide. Monterrey, NL, Mexico.
- 2003 | Mexican Council of Sci. and Tech. (CONACyT) Fellowship. Mexico City, Mexico.
- 2003 | Mexican Academy of Sciences (AMC) Research Fellowship. Mexico City, Mexico.
- 2002 | Mexican Council of Sci. and Tech. (CONACyT) National Award. Mexico City, Mexico.
- 2002 | 34th International Chemistry Olympiad. Honorific Mention. Groningen, the Netherlands.
- 2002 | XII National Chemistry Olympiad. Gold Medal. Mexican Academy of Sci. Jalapa, Mexico
- 2002 | XVI Mathematics Olympiad. Silver Medal. Mexican Academy of Sci. Oaxaca, Mexico
- 2001 | XI National Chemistry Olympiad. Gold Medal. Mexican Academy of Sci. Monterrey, Mexico
- 1997 | National Olympiad for Primary Schools. Gold Medal. Mexico City, Mexico.

## Teaching Responsibilities

- 2016 | ECH 3854: Chemical Engineering Computations (Fall, ~60 students),  
ECH 5840: Advanced Chemical Engineering Mathematics (Fall, ~20 students)
- 2015 | ECH 3854: Chemical Engineering Computations (Fall, ~60 students),  
ECH 5840: Advanced Chemical Engineering Mathematics (Fall, ~20 students)
- 2014 | Science Undergraduate Lab Internship, SULI (Berkeley National Lab, Mentor 2 students)  
Community College Internship, CCI (Berkeley National Lab, Mentor 3 students)
- 2013 | Undergraduate research program (Caltech, Mentor 4 students)
- 2011 | The nature of the chemical bond (Caltech, Teaching Assistant, 20 students)
- 2011 | Atomic-level simulations of materials and molecules (Caltech, Teaching Assistant, 15 students)
- 2010 | Summer Undergraduate Research Fellowship, SURF (Caltech, Mentor 1 student)
- 2007 | Undergraduate research program (UCLA, Mentor 1 student)

## Mentor/Advising Responsibilities

Middle School Research Advisor

2017 | Caasi Lampkin, 8th Grade (14 weeks) Rowan Ray, 7th Grade, (14 weeks)

High School Research Advisor

2016 | Taylor Bollenberg (1 semester), [2015] Judy Jo Shippen (1 semester)

Undergraduate Research Advisor

2017 | Alec P. Bigness (NSF-REU)

2016 | Alyssa Kohler, Kathryn Lopez, Jin Bae, Marlon Facey, Thiago Borges, Taylor Markley

2015 | Stephanie Marxsen, Sarah Palmon, Valdirio Segundo, Rosemary Bier, Leon Gonzalez, Sachi Kamiya

2014 | Kevin Lucht, Natasha Raghunandhan, Donna Kirk, Mohar Harjyot, Moe Aung

2013 | Alexander Aduenko, Finn Carlsvi, Yubo Su, Alex Anemogiannis  
[2010] Alan Menezes, [2007] Amanda Rees

Master Research Advisor

| Upon Request

Doctoral Research Advisor

| Upon Request

PostDoctoral Research Advisor

| Upon Request

**Thesis Committee Responsibilities**Undergraduate Thesis Committee

2016 | Constanza Miguel-Sanchez (Honors Thesis)

Doctoral Committee Member

2016 | Benjamin Crysyp (Scientific Computing), Kuan-Wen Chen (Physics)

2015 | Xuejian Chen, Divya Bahadur, Yuan Gao, James Akraasi, Xiaoshi Zhang, Chenkun Zhou, Yu Shu, Hailing Liu, Brent Bijonowski, Venroy Watson, Huihui Wang

**Departmental and University Service**

2016 | Member. Faculty Search Committee

2016 | Member. Undergraduate Committee

2015 | Member. Chemical Engineering PhD Qualifying Exam Committee.

2015 | Representative College of Engineering. The Research Computing Center (RCC) Advisory Panel. The panel consist of around 31 faculty members from a number of departments that make use of the RCC. 2015-*Current*.

**Conferences and Workshop Organization**



- 2016 | Chair. Quantum Methods. Southeastern Theoretical Chemistry Association. Florida State University, FL, USA.
- 2016 | Chair. Renewable Energy. American Vacuum Society. University of Central Florida. Orlando, FL, USA.

## Review Service

- 2017 | National Science Foundation (NSF), external reviewer  
American Chemical Society - PRF, external reviewer.
- 2016 | National Science Foundation (NSF), Panel.

## Software

- Software Developer: | ADF, QChem, Lammps, ReaxFF  
Languages: | C++, Fortran, Python, Matlab  
Operating systems: | Linux, Mac OS, Windows  
Scientific Software: | Crystal09-Crystal14-Crystal17, Vasp, QuantumExpresso, Turbomole, Jaguar, Maestro, Mathematica, ChemDraw, Macromodel, Gulp, L<sup>A</sup>T<sub>E</sub>X

## Scientific Affiliations

- 2007-2009 | American Chemical Society  
2008-2009 | American Association for the Advancement of Science  
2014-Present | American Chemical Society

## Languages

- Idioms: | English (Fluent), Spanish (Native), Mandarin (basic), French (Basic), German (Basic).