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# Jose L. Mendoza-Cortes, PhD

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## Research Interests

My research philosophy focus on attacking problems in the chemical and material sciences and developing methods needed to solve them. Some of the problems I focus on are: energy storage, ab initio electrochemistry, materials and catalysts design, chemical and crystallization mechanisms, and biomaterials. These problems are studied by using new or established methods from: accelerated dynamics, statistical mechanics, force field development, coarse grained modeling, DFT and post Hartree-Fock methods, and machine learning.

## Education

<i>Postdoc</i> , 2014	UC Berkeley/ Berkeley National Lab	Theoretical Chemistry
<i>Staff Scientist</i> , 2013	California Institute of Technology	Solid State Physics
<i>Postdoc</i> , 2013	Joint Center for Artificial Photosynthesis	Electrochemistry
<i>Ph.D.</i> , 2012	California Institute of Technology	Materials Science
<i>M.Sc.</i> , 2010	California Institute of Technology	Materials Science
<i>B.Sc.</i> , 2008	Tec de Monterrey (ITESM)	Chemistry
2006-2008	University of California, Los Angeles	Chemistry

## Current Position

09/2014–Present <i>Courtesy Professor</i>	Florida State University and Florida A&M, College of Engineering Department of Chemical and Biomedical Engineering & Materials Science and Eng.
11/2013–Present <i>Materials</i> <i>Postdoctoral Fellow</i>	Lawrence Berkeley National Laboratory & UC Berkeley Materials Science Division & Department of Chemistry Joint Center for Artificial Photosynthesis.

## Selected Publications

**Citations: 2222**, h-index: 9, Source: Google Scholar

- J. S. Kanady<sup>‡</sup>, J. L. Mendoza-Cortes<sup>‡</sup>, E. Y. Tsui, W. A. Goddard III and T. Agapie, “Oxygen Atom Transfer and Oxidative Water Incorporation in Cuboidal  $Mn_3MO_n$  Complexes based on Synthetic, Isotopic Labeling, and Computational Studies” *J. Am. Chem. Soc.*, 2013, 1073-1082. <sup>‡</sup>These authors contributed equally.
- 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  $H_2$  Uptake at 298 K” *J. Phys. Chem. Lett.*, 2012, 2671-2675.

## Selected Talks

27/03/2014 <i>Invited talk</i>	“Generation, transformation and storage of alternative energy” Energy & Materials. Chemical and Biomedical Eng. Florida State University   Florida A&M University
01/13/2014 <i>Invited talk</i>	“Generation, Transformation and Storage of Chemical Energy” Theoretical and Computational Chemistry, Department of Chemistry and Biochemistry University of California, Los Angeles

## Research Experience

2014 <i>Materials Postdoctoral Fellow</i>	<b>Lawrence Berkeley National Laboratory &amp; UC Berkeley</b> Materials Science Division & Department of Chemistry Joint Center for Artificial Photosynthesis.
2013 <i>Staff Research Scientist</i>	<b>California Institute of Technology</b> Division of Chemistry and Chemical Engineering Joint Center for Artificial Photosynthesis.
2012 – 2013 <i>Postdoctoral Fellow</i>	<b>Joint Center for Artificial Photosynthesis</b> Division of Engineering and Applied Science
2012 – 2013 <i>Postdoctoral Fellow</i>	<b>California Institute of Technology</b> Division of Chemistry and Chemical Engineering
2008 – 2012 <i>Grad. Researcher</i>	<b>California Institute of Technology</b> <i>Department of Materials Science and Applied Physics</i>
2006–2008 <i>UG Researcher</i>	<b>University of California, Los Angeles</b> Department of Chemistry and Biochemistry
2005 <i>UG Researcher</i>	<b>University of Illinois, Urbana-Champaign</b> Department of Chemistry and Biochemistry
2004–2006 <i>UG Researcher</i>	<b>Tec de Monterrey (ITESM)</b> Department of Chemistry
2003 <i>UG Researcher</i>	<b>Mexican Academy of Sciences (AMC)</b> Department of Chemistry

## Teaching Experience

2014 <i>Mentor</i>	<b>Science Undergraduate Laboratory Internship (SULI)</b> 2 undergraduate students – Lawrence Berkeley National Laboratory
2014 <i>Mentor</i>	<b>Community College Internship (CCI)</b> 3 undergraduate students – Lawrence Berkeley National Laboratory
2012–2013 <i>Co-Mentor</i>	<b>Graduate research program</b> 2 grad students – California Institute of Technology
2013 <i>Co-Mentor</i>	<b>Undergraduate research program</b> 4 undergraduate students – California Institute of Technology
2011 <i>Teaching Assistant</i>	<b>The nature of the chemical bond</b> 15 students – California Institute of Technology
2010 <i>Teaching Assistant</i>	<b>Atomic-level simulations of materials and molecules</b> 15 students – California Institute of Technology.
2010 <i>Co-Mentor</i>	<b>Summer Undergraduate Research Fellowship (SURF)</b> 2 undergraduate students – California Institute of Technology
2007 <i>Mentor</i>	<b>Undergraduate research program</b> 1 student – University of California, Los Angeles

## Leadership Experience

02/2009–02/2012 <i>President</i>	<b>Caltech's Club Latino</b> Organized cultural events along with grads, undergrads and the diversity administration such as Semana Latina and the World's Fair Festival.
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09/2009–09/2011  
*Board of Directors*

**Caltech's Graduate Student Council**

Part of the steering, academics and advocacy committees to provide support, resources and voice to underrepresented student groups.

## Publications

**Citations: 2222**, h-index: 9, Source: Google Scholar

### In Press (Research Articles)

- J. L. Mendoza-Cortes, Q. An, W. A. Goddard, S. Zybin, "The importance of molecular dipole in the packing of molecular solids: The case of Tetrazino-tetrazine-tetraoxide (TTTO)" *J. Comp. Chem.*, **2014**, accepted.
- 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*, *2014*, <sup>‡</sup>These authors contributed equally.
- N. Nair, J. L. Mendoza-Cortes, R. Abrol, W. A. Goddard and V. Prakash Reddy, "Observation of tetrafluorobenzynes radical cation and trifluorobenzynes cation by CID-mass spectrometry" *Journal of Organometallic Chemistry*, *2013*, 133-139.
- J. S. Kanady<sup>‡</sup>, J. L. Mendoza-Cortes<sup>‡</sup>, E. Y. Tsui, W. A. Goddard III 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" *J. Am. Chem. Soc.*, *2013*, 1073-1082. <sup>‡</sup>These authors contributed equally.
- 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" *J. Phys. Chem. Lett.*, *2012*, 2671-2675.
- 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" *J. Phys. Chem. A*, *2012*, 1621-1631.
- J. L. Mendoza-Cortes, Tod A. Pascal and W. A. Goddard, "Design of Covalent Organic Frameworks for Methane Storage" *J. Phys. Chem. A*, *2011*, 13852-13857.
- 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" *J. Phys. Chem. A*, *2010*, 10824-10833.
- S. S. Han, J. L. Mendoza-Cortes and W. A. Goddard, "Recent advances on simulation and theory of hydrogen storage in metal-organic frameworks and covalent organic frameworks" *Chem. Soc. Rev.*, *2009*, 1460-1476.
- D. J. Tranchemontagne, J. L. Mendoza-Cortes, M. O'Keeffe and O. M. Yaghi, "Secondary building units, nets and bonding in the chemistry of metal-organic frameworks" *Chem. Soc. Rev.*, *2009*, 1257-1283.
- H. M. El-Kaderi, J. R. Hunt, J. L. Mendoza-Cortes, A. P. Cote, R. E. Taylor, M. O'Keeffe and O. M. Yaghi, "Designed synthesis of 3D covalent organic frameworks" *Science*, *2007*, 268-272.
- J. L. Mendoza, H. M. El-Kaderi, J. R. Hunt, A. P. Cote and O. M. Yaghi, "Covalent Organic Frameworks" *Abs. of Papers of the Am. Chem. Soc.*, *2007*, 438-438.
- 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>)" *Abs. of Papers of the Am. Chem. Soc.*, *2007*, 291-291.
- 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" *J. Org. Chem.*, *2005*, 10198-10201.

### In Press (Book Chapters and Other Publications)

- 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.
- 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

- J. L. Mendoza-Cortes, Martin Head-Gordon “Selectivity in the reduction of CO<sub>2</sub> to CO using quantum mechanical methods” J. Phys. Chem. C, 2015, in preparation.
- J. L. Mendoza-Cortes\*, Nahid P. Khiabani, “Two levels of complexity for multivariate MOFs: MOF 2000” Proc. Natl. Acad. Sci., 2015, in preparation.
- Nahid P. Khiabani, J. L. Mendoza-Cortes\*, “The Oil/Water interface: The effect of counter ions for oil recovery” Proc. Natl. Acad. Sci., 2015, in preparation.
- J. L. Mendoza-Cortes\*, Alexander A. Aduenko, “Understanding La<sub>1-x</sub>Ca<sub>x</sub>CoO<sub>3</sub> for fuel cells reaction: Oxygen-Evolution Reaction (OER) and Oxygen-Reduction Reaction (ORR)” J. Phys. Chem. Lett., 2015, in preparation.
- J. L. Mendoza-Cortes\*, “Thermodynamic stability and electronic properties of all phases of WO<sub>3</sub> for light capture and conversion” Energy & Environmental Science, 2015, in preparation.
- J. L. Mendoza-Cortes\*, “Recent Advances in Molecular Simulation of Adsorption” Molecular Simulation (invited review), 2015, in preparation.
- J. L. Mendoza-Cortes\*, “Origin of the positive cooperativity in the template-directed formation of molecular machines” J. Phys. Chem. A, 2015, in preparation.
- J. L. Mendoza-Cortes\*, Yubo Su, “H<sub>2</sub> uptake at room temperature of frameworks that exceeds DOE volumetric standards” J. Am. Chem. Soc., 2014, in preparation.
- J. L. Mendoza-Cortes, S. Bajaj, Q. An, W. A. Goddard, S. Zybin, and T. M. Klapotke, “Prediction of crystal packing for the new high energy molecule: Bistetrazole-tetraoxide (BTTO)” J. Phys. Chem. C, 2014, in preparation.
- J. L. Mendoza-Cortes\*, Alexander A. Aduenko, “Generalization of the sorption process of porous materials”, arXiv, 2014

### Research Grants

6. J. L. Mendoza-Cortes, Alexander G. Anemogiannis “Molecular Dynamics Approach to Finding New Hydroxide Conducting Membranes to be Implemented in Artificial Photosynthetic Cells”, Proposal, 2013 (USD \$280K/2 years).
5. J. L. Mendoza-Cortes “High-throughput First Principles In Silico Screening to Predict Optimum Band Gap and Stability for Light Capture in Solar Fuel Generation”, Proposal, 2013 (USD \$280K/2 years).
4. H. Furukawa; J. L. Mendoza-Cortes; O. M. Yaghi; W. A. Goddard, “A new form of hydrogen storage inside porous frameworks”, Proposal, 2011 (USD \$3M/4 years).
3. D. Benitez; J. L. Mendoza-Cortes; F. Stoddart; W. A. Goddard, “Borromean Ring Metallic Organic Framework systems for molecular nanomachines”, Proposal, 2010 (USD \$1M/2 years).
2. J. L. Mendoza-Cortes; W. A. Goddard; J. K. Kang, “Development of New Materials and Techniques for CO<sub>2</sub> Utilization and Storage for Clean industry”, Proposal, 2009 (USD \$4M/4 years).
1. H. Furukawa; J. L. Mendoza-Cortes; O. M. Yaghi; W. A. Goddard, “A Joint Theory and Experimental Project in the High-Throughput Synthesis and Testing of Porous COF and ZIF Materials for On-Board Vehicular Hydrogen Storage”, Accepted DOE grant, 2008-2013 (USD \$2M/5 years).

## Selected Invited Talks and Presentations

27/03/2014 <i>Invited talk</i>	“Generation, transformation and storage of alternative energy” Energy & Materials, Chemical and Biomedical Engineering Florida State University   Florida A&M University
01/13/2014 <i>Invited talk</i>	“Generation, Transformation and Storage of Chemical Energy” Theoretical and Computational Chemistry, Department of Chemistry and Biochemistry University of California, Los Angeles
11/14/2013 <i>Keynote speaker</i>	“High performance nanostructured materials for hydrogen storage” 10th International Symposium of New Materials for electrochemical systems Dept. of Chemistry, Instituto Politecnico Nacional - CINVESTAV
11/09/2013 <i>Invited talk</i>	“Artificial Photosynthesis; a path to alternative energy” <i>Latino students: 3rd annual Adelante Young Men (AYM) conference</i> Pasadena Youth Center and Pasadena City College
10/16/2013 <i>Invited talk</i>	“Large scale ab initio calculations for excited states and light conversion” <i>Special Seminar on photoexcited systems</i> Dept. of Chemistry, Harvard University
10/01/2013 <i>Invited talk</i>	“A first principles approach to energy storage and conversion” <i>Special Seminar on photoactivated systems and nanoporous materials</i> Dept. of Chemistry, University of Minnesota, Twin cities
03/25/2013 <i>Invited talk</i>	“Production and Storage of Renewable Clean Energy from First Principles” <i>Special Seminar on Computational Materials Sci. and Materials Modeling</i> Dept. of MatSci and MechE, University of Maryland, College Park
10/31/2012 <i>Invited talk</i>	“Trapping/storing gases in porous organic and metal-organic materials” <i>Special Fellows Conference Series</i> Dept. of Engineering, Tenaris University
09/14/2009 <i>Poster presentation</i>	“Hydrogen storage in Covalent & Metal-Organic Frameworks” <i>Ab Initio Modelling in Solid State Chemistry</i> Dept. of Chemistry, Imperial College of London
09/06/2009 <i>Poster presentation</i>	“Methane storage in Covalent & Metal-Organic Frameworks” <i>Workshop in Ab Initio Solid State Chemistry</i> Dept. of Chemistry, University of Torino
06/22/2009 <i>Poster presentation</i>	“Gas storage in microporous Materials” <i>Summer School on the Fundamental of Neutron Scattering</i> NIST Center for Neutron Research (NCNR)
07/28/2008 <i>Poster presentation</i>	“Covalent Organic Framework as outstanding methane storage materials” <i>Summer School on Periodic Structures and Crystal Chemistry</i> Dept. of MatSci, University of California, Santa Barbara
03/25/2007 <i>Poster presentation</i>	“Covalent Organic Frameworks” <i>American Chemical Society, National Convention</i> American Chemical Society

## Honors and Awards

2009 <i>15 fellows worldwide</i>	Roberto Rocca Graduate Fellowship Awarded on the basis of the student’s academic and professional accomplishments. Buenos Aires, Argentina
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2008 <i>13 fellows worldwide</i>	International Center for Material Research(ICMR) fellowship Best Poster award from the ICMR School on Periodic Structures and Crystal Chemistry. UCSB, Santa Barbara, CA, USA. Declined.
2007 <i>Best paper of the year in Science magazine</i>	AAAS Newcomb Cleveland Prize 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 <i>Poster award</i>	UCLA Glenn T. Seaborg Symposium Contest of posters among all graduate students and postdocs in the Department of Chemistry and Biochemistry in UCLA. Los Angeles, CA, USA
2006 <i>Young scientist award</i>	Mexican Ministry of Education – SEP For contributions to the advancement of science and leadership potential on the field of expertise. Mexico City, Mexico
2005 <i>Research scholarship</i>	Snyder Research Fellowship – UIUC Fellowship to support undergraduate students research at the University of Illinois at Urbana-Champaign. Advisor: Prof. Jeffrey S. Moore. Urbana, Illinois, USA
2004 <i>20 fellows nationwide</i>	Xorge A. Dominguez Fellowship Fund created by Dr. Javier Rivas Ramos to promote the advancement of pure and applied chemistry. Monterrey, NL, Mexico
2004 <i>30 fellows nationwide</i>	Council of Science and Technology (CONACYT) fellowship National fellowship given to winners of the national and international sciences Olympiads. Mexico City, Mexico
2003 <i>Research fellowship</i>	National Academy of Science (AMC) Fellowship National Academy of Sciences. Monterrey, Mexico.
2002 <i>National Award</i>	Council of Science and Technology (CONACYT)'s national award For academic achievements. Oaxaca, Mexico.
2002 <i>Honoric mention</i>	34th International Chemistry Olympiad University of Groningen. Groningen, the Netherlands
2002 <i>Gold medal</i>	XII National Chemistry Olympiad Mexican Academy of Sciences. Jalapa, Veracruz, Mexico
2002 <i>Silver medal</i>	XVI National Mathematics Olympiad Mexican Academy of Sciences. Oaxaca, Oaxaca, Mexico
2001 <i>Gold medal</i>	XI National Chemistry Olympiad Mexican National Academy of Sciences. Monterrey, NL, Mexico
1997 <i>Gold medal</i>	National Olympiad of Knowledge for Primary Schools The President of Mexico received the medalists. Mexico City, Mexico

## Computer Skills

Software Developer:	ADF, QChem, Lammmps, ReaxFF
Languages:	C++, Fortran, Python, Matlab
Operating systems:	Linux, Mac OS, Windows
Scientific Software:	Crystal09-14, 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 (Very basic).