David Mora Fonz

Chemistry, Physics, Materials Science, Data Science

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I am interested in using atomistic modelling techniques to study materials for energy applications, electronics and catalysis. My main interests can be summarised under the headings of ab initio methods, force fields development, metal oxides, amorphous materials, surface science, catalysis, data science and global optimisation methods. More recently, I have been working on the local government on energy-related matters and as an Advisor for the Secretariat for Energy Development in Tabasco, Mexico.

Brief CV

2022 **Head of the Energy and Technologies Department**, *Centro Municipality*, Tabasco, Mexico.

2021–2022 **Sub-coordinator of Development, Research & Technologies**, *Centro Municipality*, Tabasco, Mexico.

2020–2022 **Advisor**, *Secretariat for Energy Development*, Tabasco, Mexico.

2020 **Honorary Postdoctoral Research Associate in the group of Professor Alexander L. Shluger**, *University College London*, London, UK.

2017–2020 **Postdoctoral Research Associate in the group of Professor Alexander L. Shluger**, *University College London*, London, UK.

2016–2017 **Postdoctoral Researcher in the group of Professor Sir C. Richard A. Catlow**, *University College London*, London, UK.

2012–2016 **PhD in Computational Chemistry**, *University College London*, London, UK.

2010 **BSc, Chemical Engineering**, *Juarez Autonomous University of Tabasco (UJAT)*, Cunduacán, Mexico.
Grade 98.5/100, graduated with honours, highest grade from over 100 students

Languages

- Spanish - Native speaker
- English - Fluent

Teaching Experience

- "Physical chemistry for undergraduate students", 2009 (48 h), UJAT, Mexico
- "Thermodynamics for undergraduate students", 2009 (48 h), UJAT, Mexico
- "Mass and Energy Balances for undergraduate students", 2009 (48 h), UJAT, Mexico
- "Chemical kinetics and catalysis", 2009 (48 h), UJAT, Mexico
- "Quantum Physics", 2018-2019, UCL, UK

Reviewing & Editing Duties

- Reviewer: Nature Communications, Journal of the American Chemical Society, Physical Review Materials, Physical Review B, ACS Applied Materials & Interfaces, Solid State Communications, Frontiers in Materials, physica status solidi (b)

- Editor: Catalysis Today

Research Visits

2022 Research visit to the group of Dr Alexey Sokol in the Chemistry Department at UCL. The project was focused on the development of force fields.

2018 Research visit to the group of Professor Christian Schön in the Max Planck Institute, Stuttgart, Germany. The project was focused on development, using experimental and DFT data, of new interatomic potentials and exploration of energy landscapes

2015 Research visit to the group of Professor Stefan T. Bromley in the Institute of Theoretical and Computational Chemistry at the University of Barcelona (IQTCUB). The project was focused on fitting new Cu/ZnO interatomic potentials to DFT data (1 month)

2010 "Student Mobility" program, Catalysis Investigation Unit (UNICAT), UNAM, Mexico (8 months)

2010 Summer of the scientific research, Catalysis Investigation Unit (UNICAT), UNAM, Mexico (2 months)

2008 Summer of the scientific research, Catalysis Investigation Unit (UNICAT), UNAM, Mexico (2 months)

Publications

2020 **David Mora-Fonz**, Moloud Kaviani, and Alexander L. Shluger (2020). "Disorder-induced electron and hole trapping in amorphous TiO_2 ". In: *Physical Review B* 102.5, p. 054205. DOI: 10.1103/PhysRevB.102.054205.

2020 **David Mora-Fonz**, J. Christian Schön, Janett Prehl, Scott M. Woodley, C. Richard A. Catlow, Alexander L. Shluger, and Alexey A. Sokol (2020). "Real and Virtual Polymorphism of Titanium Selenide with Robust Interatomic Potentials". In: *Journal of Materials Chemistry A* 8.28, pp. 14054–14061. DOI: 10.1039/D0TA03667F.

2020 **David Mora-Fonz** and Alexander L. Shluger (2020). "Modeling of Intrinsic Electron and Hole Trapping in Crystalline and Amorphous ZnO". In: *Advanced Electronic Materials* 6.1, p. 1900760. DOI: 10.1002/aelm.201900760.

2020 Michael Higham, **David Mora-Fonz**, Alexey A. Sokol, Scott M. Woodley, and C. Richard A. Catlow (2020). "Morphology of Cu Clusters Supported on Reconstructed Polar ZnO (0001) and (000$\bar{1}$) Surfaces". In: *Journal of Materials Chemistry A*. DOI: 10.1039/D0TA08351H.

2020 Naoki Ohashi, **David Mora-Fonz**, Shigeki Otani, Takeshi Ohgaki, Masashi Miyakawa, and Alexander Shluger (2020). "Inverse Perovskite Oxysilicides and Oxygermanides as Candidates for Nontoxic Infrared Semiconductor and Their Chemical Bonding Nature". In: *Inorg. Chem.* 59.24, pp. 18305–18313. DOI: 10.1021/acs.inorgchem.0c02897.

2019 **David Mora-Fonz** and Alexander L. Shluger (2019). "Making amorphous ZnO: Theoretical predictions of its structure and stability". In: *Physical Review B* 99.1, p. 014202. DOI: 10.1103/PhysRevB.99.014202.

2018 Qing Hou, John Buckeridge, Tomas Lazauskas, **David Mora-Fonz**, Alexey A. Sokol, Scott M. Woodley, and C. Richard A. Catlow (2018). "Defect formation in In_2O_3 and SnO_2: a new atomistic approach based on accurate lattice energies". In: *Journal of Materials Chemistry C*, pp. 12386–12395. DOI: 10.1039/C8TC04760J.

2018 Tomas Lazauskas, Alexey A Sokol, John Buckeridge, C Richard A Catlow, Susanne G E T Escher, Matthew R Farrow, **David Mora-Fonz**, Volker W Blum, Tshegofatso M Phaahla, Hasani R. Chauke, Phuti E. Ngoepe, and Scott M. Woodley (2018). "Thermodynamically accessible titanium clusters Ti_N, $N = 2$–32". In: *Physical Chemistry Chemical Physics* 20.20, pp. 13962–13973. DOI: 10.1039/C8CP00406D.

2017 Matthew R. Farrow, John Buckeridge, Tomas Lazauskas, **David Mora-Fonz**, David O. Scanlon, C. Richard A. Catlow, Scott M. Woodley, and Alexey A. Sokol (2017). "Heterostructures of GaN with SiC and ZnO enhance carrier stability and separation in framework semiconductors". In: *Physica Status Solidi A* 214.4, p. 1600440. DOI: 10.1002/pssa.201600440.

2017 **David Mora-Fonz**, C. Richard A. Catlow, Matthew R. Farrow, Tomas Lazauskas, Scott M. Woodley, and Alexey A. Sokol (2017). "Why Are Polar Surfaces of ZnO Stable?" In: *Chemistry of Materials* 29.12, pp. 5306–5320. DOI: 10.1021/acs.chemmater.7b01487.

2017 **David Mora-Fonz**, Tomas Lazauskas, Stefan T. Bromley, C. Richard A. Catlow, Scott M. Woodley, and Alexey A. Sokol (2017). "Development of Interatomic Potentials for Supported Nanoparticles: The Cu/ZnO Case". In: *The Journal of Physical Chemistry C* 121.31, pp. 16831–16844. DOI: 10.1021/acs.jpcc.7b04502.

2015 Andrew J. Logsdail, **David Mora-Fonz**, David O. Scanlon, C. Richard A. Catlow, and Alexey A. Sokol (June 2015). "Structural, Energetic and Electronic Properties of (100) Surfaces for Alkaline Earth Metal Oxides as Calculated with Hybrid Density Functional Theory". In: *Surface Science* 642, pp. 58 –65. DOI: 10.1016/j.susc.2015.06.012.

2015 **David Mora-Fonz**, John Buckeridge, Andrew J. Logsdail, David O. Scanlon, Alexey A Sokol, Scott M. Woodley, and C. Richard A. Catlow (2015). "Morphological Features and Band Bending at Non-Polar Surfaces of ZnO". In: *The Journal of Physical Chemistry C* 119.21, pp. 11598–11611. DOI: 10.1021/acs.jpcc.5b01331.

2014 Catherine Brookes, Peter P. Wells, Nikolaos Dimitratos, Wilm Jones, Emma K. Gibson, David John Morgan, Giannantonio Cibin, Chris Nicklin, **David Mora-Fonz**, David O. Scanlon, C. Richard A. Catlow, and Mike Bowker (Nov. 2014). "The Nature of the Molybdenum Surface in Iron Molybdate. The Active Phase in Selective Methanol Oxidation". In: *The Journal of Physical Chemistry C* 118.45, pp. 26155–26161. DOI: 10.1021/jp5081753.

Conferences and Meetings

Meetings

- "Energy efficiency and decarbonization in Industry and Buildings", *Climate and Energy collaboration programme (DEPP III), Copenhagen, Denmark* (August 27 to September 4, 2022)

Oral presentations

- **Invited.** "Superficies, Desorden y Fase Amorfa del ZnO", *Coloquio Semanal, ICAT-UNAM, Mexico* (January, 2020)
- "Theoretical Modeling of Intrinsic Charge Trapping in Crystalline and Amorphous ZnO", *International Materials Research Congress, Cancun, Mexico* (August, 2019)
- **Invited.** "Why are polar surfaces of Zinc Oxide stable?", *International Materials Research Congress, Cancun, Mexico* (August, 2019)
- **Invited.** "Doing Chemistry with Computers", *Paul Dirac Talk, Prometeo Institute, Tabasco, Mexico* (August, 2019)
- **Invited.** "From Chess to Science", *Injudet Youth Week Seminar, Tabasco, Mexico* (August, 2019)
- **Invited.** "Surface disorder and amorphous phase of ZnO", *Seminar at the Nanoscale Science Department, Max Planck Institute for Solid State Research in Stuttgart, Germany* (April, 2019)
- "Modelling of Charge Trapping in Amorphous ZnO", *International Workshop on Zinc Oxide and other Oxide Semiconductors, Warsaw, Poland* (September, 2018)
- "Amorphous ZnO: Structure, Electronic Properties and Charge Trapping", *International Materials Research Congress, Cancun, Mexico* (August, 2018)
- "The Study of ZnO Surfaces Using Computational Techniques", *2016 Innovation Match, Guadalajara, Jalisco, Mexico* (April 2016)
- "Explaining the Stability of the Polar Surfaces of ZnO Using Interatomic Potentials", *MCC 2nd Conference, Cardiff University, Cardiff, UK* (April 2016)
- "A Theoretical Study in the Stability of the Polar Surfaces of ZnO", *2015 MRS Fall Meeting, Boston, Massachusetts, USA* (December 2015)
- "A Hybrid DFT Study on the Morphological Features and Band Bending at the $(10\bar{1}0)$ and $(11\bar{2}0)$ ZnO Surfaces", *2015 MRS Fall Meeting, Boston, Massachusetts, USA* (December 2015)
- "Surface Reconstructions at Polar Surfaces of ZnO", *The 46th Annual BACG Conference, Queen Mary University, London, UK* (June 2015)
- "Stability of ZnO Polar Surfaces", *EMRS Meeting, Warsaw, Poland* (September, 2014)
- "A DFT Study of the MoO_3/Fe_2O_3 System: a Model Catalyst for the Formaldehyde Synthesis", *International Materials Research Congress, Cancun, Mexico* (August, 2014)
- "Why are Polar Surfaces of ZnO Stable?", *International Conference on the Physics of Semiconductors, Austin, Texas* (August, 2014)
- "A Study of the Nonpolar $(10\bar{1}0)$ and $(11\bar{2}0)$ ZnO Surfaces and a Stabilisation Mechanism for the Polar (0001)-Zn Surface", *Renewable Energy and Solid-State Chemistry Conference, Mansfield, UK* (April, 2014)
- "CO_2 Hydrogenation for Methanol Synthesis", *National Congress of Chemical Engineering, Villahermosa Tabasco, Mexico* (August 2012)
- "Computational Modelling Studies in the Hydrogenation of CO_2 for Methanol Synthesis", *National Congress of Science, Cunduacán Tabasco, Mexico* (August 2012)

Poster Presentations

- "Modelling Amorphous ZnO: Structure and Electronic Properties", *International Conference on the Physics of Semiconductors, Montpellier, France* (July, 2018)
- "An *ab-initio* Approach in the Geometry and Electronic Structure of Nonpolar ZnO Surfaces", *EMRS Spring Meeting, Lille, France* (May 2015)
- "Stability of ZnO Polar Surfaces", *Departmental Postgraduate Poster Session, University College London, UK* (June 2014)
- "Knowledge-Led Master Code. An Automation Tool for Computational Scientists", *RSC Solid State Christmas Conference, Bath, UK* (November 2013)

- "HDS of 4,6-DMDBT with NiMoP Catalysts Supported on Alumina. Effect of the Incorporation Method of P", *National Expo-Sciencies, Puebla, Mexico* (October 2008)
- "HDS of 4,6-DMDBT with NiMoP Catalysts Supported on Alumina. Effect of the Incorporation Method of P", *Chemistry Forum, Juarez Autonomous University of Tabasco, Mexico* (November 2008)

Awards and Scholarships

- Danida Fellowship Center: "Energy Efficiency and Energy Management in Buildings and Industry", Copenhagen, Denmark, 2022
- National Researcher Level 1 in the National System of Researchers-CONACyT (Mexico), 2020-2022
- Member of the European Cooperation in Science and Technology, Action CM1104 (Reducible oxide chemistry, structure and functions), Working Group 2 (Synthesis and Characterisation), 2015-present
- Dean's Prize by the Faculty of Mathematical and Physical Sciences at UCL (UK), ∼£5,000/year, 2012-2015
- SEP (Mexico) scholarship holder, ∼£3,750/year, 2013-2015
- CONACyT (Mexico) scholarship holder, ∼£25,000/year, 2012-2016
- UJAT (Mexico) scholarship holder, ∼£5,200/year, 2012-2016
- First place poster presentation, Chemistry Forum 2008, Cunduacán Tabasco, UJAT, November 2008
- Scholarship from the Mexican program "Becanet" to distinguished students, ∼£500, 2009
- Scholarship from the TELMEX foundation, ∼£420/year, 2006-2010
- Scholarship recipient from the "National Scholarship Program", ∼£600/year, 2002-2009
- Sport scholarship from the Tabasco Institute for the Youth and Sport (INJUDET), ∼£300/year, 1994-2005

Extra-Curricular Activities

- First board player, representing UCL, in the British Universities' Chess Association Championship, Birmingham, UK, 2014-2016
- Best Mexican player under 18, World Youth Chess Championship, Belfort France, July 2005
- 5 times national chess champion in Mexico
- 8 times second place in national chess championships in Mexico
- 6 times third place in national chess championships in Mexico
- More than 40 participations in national and international chess tournaments
- International chess player since 2005
- Mexican national chess player since 1994
- Current FIDE rating: 2147