Álvaro Vázquez-Mayagoitia | CV

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Data driven chemistry and materials scientist,
HPC specialist

Summary

I am a computational scientist with >18 years of experience in large scale scientific simulations, with a background in computational chemistry and parallel programming. I contribute to notable electronic structure codes for HPC systems to operate in the largest US DOE.gov computing facilities. In a typical day, I do computational science consulting for national and international scientific projects in areas such as quantum chemistry, materials science, molecular dynamics and data science, which has led to scientists on those project teams publishing dozens papers in high impact journals, including Science, Nature, and PRL. I have authored and co-authored more than 55 refereed papers, book chapters, and technical reports; and more are in progress. My publications have received over 2,280 citations (in Google Scholar). I service as reviewer for DOE.gov grants and allocation proposals, and for relevant journals in my science domain.

Employment History

Current Appointment.....

- **Argonne National Laboratory** — **Lemont, IL**
  Computational Scientist, Computational Science Division — *August 2019– present*

  Contribute to enhancing parallel electronic structure codes for exascale era architectures. Developer of NwchemEX. GPU development using SYCL, OpenMP and CUDA. Co-PI of quantum chemistry and materials science grant proposals. POC of two Early Science Program projects for Aurora next DOE's exascale computer. Deploy AI/ML models and complex workflows for data-driven materials discovery. Contributor of IGEN organization to foster under represented communities in physical sciences graduate programs. Career mentor and supervisor of ALCF postdocs. Communicate research advances in national and international conferences and in high impact publications. AI/data driven science capabilities lead at CPS Division.

- **University of Chicago** — **Chicago, IL**
  Senior Scientist, CASE — *January 2020– present*

  Join appointment affilitated to University of Chicago Consortium for Advanced Science and Engineering (UChicago CASE). Participate in external funding proposals, such as NSF and NHI. Mentor students, postdocs and early-career staff. Collaborate in research programs in chemistry, physics, materials sciences, and computer science.

Previous Employment

- **Argonne National Laboratory** — **Lemont, IL**
  Assistant Computational Scientist, Computational Science Division — *July 2013– July 2019*

  Contributed enhancing parallel electronic structure codes, including NWChemEX, NWChem, MADNESS, Quantum Expresso, BigDFT and FHI-aims. Provided consulting and review for projects to use extreme-scale computing efficiently in Theta, a 10 petaflop Intel KNL based Cray/XC40 machine. Co-PI of quantum chemistry and materials science projects. Contributed to grant writing and reporting. Collaborated to provide performance estimations and give technical advise for non-recurring engineering contracts for next-generation supercomputers. Contributed to Argonne Leadership Computing Facility (ALCF) Data Science Program deploying machine learning approaches and complex work-flows to accelerate materials discovery. Contributed to advancements in predicting organic dyes to improve solar cells, and in the study of inner forces within molecular crystals with applications in medicine and electronics. Led the ALCF Postdoctoral Committee, where I manage the recruitment and hiring of postdoctoral researchers. Mentored ALCF postdocs to ensure they are developing the skills and experience needed to advance their careers. Presented original research in national and international conferences, publish in high impact publications.

- **Argonne National Laboratory** — **Lemont, IL**
  Postdoctoral Appointee, Argonne Leadership Computing Facility — *March 2011–July 2013*

  Ported and optimized codes for the second generation of ALCF's 10 petaflop supercomputers, Mira IBM/Q. Coded in MADNESS (*C++11*/MPI/Pthreads), a wavelet-base base code, enabling large systems simulations for chemical catalysis and strategic applications for new and clean fuels. I was the original author in MADNESS of: libXC interface for DFT functionals, geometry optimization, Coupled Perturbed Hartree-Fock method, frequency dependent dipole polarizabilities and parallel algebra routines. Enhanced NWCHEM with new functionals and wavefuntion methods, dispersion corrections, Hirshfeld population analysis, reactivity indexes, geometry coordinate conversions, Raman spectra and python interfaces for ab-initio molecular dynamics. Supervised Research Aides. Collaborated on writing grant proposals. Contributed creating curated data sets of organic molecules for machine learning.

- **Scuola Normale Superiore** — **Pisa, Italy**
  Postdoctoral Research — *No taken*

  Project awarded to develop massive parallel anharmonic vibrational studies of metal-organic complexes.

- **Chemical Sciences Division** — **Oak Ridge, TN**
  Postdoctoral Research Assistant — *No taken*

  Position to contribute in computational design of actinide-lanthanide separation agents for nuclear waste management.

- **Oak Ridge National Laboratory/U. Tennessee/ JICS** — **Oak Ridge, TN**
  Postdoctoral Research Assistant — *September 2008– December 2010*

  Carried out research in molecular interactions driven by dispersion forces. Implemented and validated semi-empirical and double-hybrid DFT functionals, and did an extensive comparison with correlated methods, such as MP2 and Coupled Cluster. Investigated the structure, interactions, and electronic properties of DNA bases analogues extended with fused ring and substituted with selenium atoms. Conducted research on the formation of biomolecules in early earth environments to support life origin theories. Developed Raman spectra simulations by combining linear response theory and finite differences in the resonance and non-resonance regimes. Indeed, my Raman implementation used multi parallelism for massive computations in petascale computers. Coded linear response theory in MADNESS a wavelet code. Published 7 peer-reviewed papers, delivered oral presentations in major chemistry conferences.

- **Universidad Autónoma Metropolitana** — **México City**
  Postdoctoral Research (short-term) — *May 2008–August 2008*

  Developed subroutines in NWChem to compute the semi empirical dispersion energy contribution in Density Functional simulations in the Kohn-Sham scheme.

Education

Academic Qualifications

- **Universidad Autónoma Metropolitana** — **México City**
  PhD in Chemical Sciences, Scores: 95/100. — *2003–2008*
- **Universidad Autónoma Metropolitana** — **México City**
  BS in Chemistry, Scores: 90/100. — *1997–2003*

Awards

- **National Mexican Council of Science and Technology**
  PhD studies fellowship , Joined the certified Physical Chemical Theory graduate program. — *2003-2008*
- **Oak Ridge National Laboratory**
  ASTRO fellowship/ORAU/ORISE, Summer research experience to complete PhD research — *2006*
- **National Mexican Council of Science and Technology.**
  Travel grant, Funding to attend international conferences and visit US research groups. — *2003*
- **Universidad Autónoma Metropolitana**
  Academic Excellence Medal, Undergrad studies. — *2003*
- **Universidad Autónoma Metropolitana**
  Undergrad fellowship, Contributed to original research in quantum chemistry. — *2001*

Notable PhD Projects

- Developed subroutines to optimize Potential Energy Surface corrected of Basis Set Superposition Error.
- Studied the stability of double negative charged chemical species in gas phase and in solution.
- Solvent effects on electronic structure of charged systems.
- Investigated the effect of self-interaction in the correct vanishing of orbital densities in atoms and molecules.
- Analysis of regio-selectivity for electrophilic attack in reduced quinones.
- Studied of the effect of exact-exchange in energy gap of frontier orbitals.
- Developed subroutines to evaluate the population analysis with the stock-holder approach (Hirshfeld and Hirshfeld-I) in NWChem.

Synergistic Activities

August 2018	co-organizer of MOLSSI funded workshop: "Solving or Circumventing Eigenvalue Problems in Electronic Structure Theory".
Since 2016	Chair of the ALCF postdoctoral committee, member of the CELS division postdoctoral committee and Named Fellowship review committee program
Since 2015	co-PI ELSI - Infrastructure for Scalable Electronic Structure Theory.
Since 2009	Member of the National Mexican National Council of Science and Technology in (SNI level I, practicing abroad).
Service	Reviewer for Journals and Grant Proposals including The Journal Physical Chemistry Letters, Journal Chemical Physics, International Journal of Modern Physics B, Letters in Organic Chemistry, Royal Chemical Society, among others.

Research Grants

- 2020-051-R1 Eugene Yang (PI) 1/May/2020 - 30/Sep/2020 DOE, Office of Science (Laboratory Directed Research and Development) *Predict PFAS toxicity with deep learning approaches* The goal of this project is to predict the toxicity of poly and per-fluorinated compounds (PFAS) using deep learning. This work include processing and fragment recognition of chemical fragments that lead to high toxicity of PFAS. Role: Co-PI.
- 2017-034-R1 Marius Stan (PI) 1/Oct/2016 - 30/Sep/2018 DOE, Office of Science (Laboratory Directed Research and Development) *Perfect Thermodynamics of Imperfect Materials* This project aims at understanding and predicting formation and stability/metastability of highly defective, non-stoichiometric transition metal oxide material phases, via theory, intelligent computer simulations, and advanced experiments. Role: Co-PI.
- NSF Award: 1450280 Volker Blum (PI) 1/Oct/2015 - 30/Sep/2019 NSF, *SI2-SSI: ELSI – Infrastructure for Scalable Electronic Structure Theory*, This proposal is to consolidate some existing linear parallel libraries to compute eigenvalues and eigenvectors of large dense and sparse matrices for electronic structure codes. Role: Co-PI.
- 2014-139-N0 Al Wagner (PI) 10/01/2014-9/30/2016 DOE, Office of Science (Laboratory Directed Research and Development): *Fast Electronic Structure Methods for Rapid Reaction Screening for Inorganic Materials Synthesis and Particle Formation* This proposal is to develop a highly parallelized semi-empirical molecular orbital (SEMO) and semi-empirical density functional theory based tight binding (TB-DFT) codes to enable the discovery of new synthesis pathways via simulations involving up to tens of thousands of atoms for molecules and solids. Role: Co-PI.
- 2013-199-R1 Nichols Romero (PI) 10/01/2013-9/30/2015 DOE, Office of Science (Laboratory Directed Research and Development) *MADNESS for Material* This proposal aims to develop a DFT software for Materials research within the wavelets code MADNES using petaflop super computers. Role: Co-PI.
- 2013-212-R1 Alvaro Vazquez-Mayagoitia (PI) 10/01/2013-9/30/2015 DOE, Office of Science (Laboratory Directed Research and Development): *Multiscale Materials Modeling using Accurate Ab Initio Approaches (M3A3)* This proposal is to develop and research Machine Learning approaches for multiscale methods in computational simulations of large materials simulations. Role: PI.

Graduate and Postdoctoral Advisees

Laura Ratcliff (ANL, co-mentored postdoc), Erwin Garcia Hernandez (Universidad Autonoma Metropolitana, grad intern), Yukina Yokoi (Toyohashi University, grad intern), Ganesh Sivaraman (ANL, postdoc), Abhishek Bagusetti (ANL, postdoc) Colleen Bertoni (ANL, short period co-mentored postdoc)

Technical and Personal skills

- **Programming Languages:** Proficient in: Fortran77/90, C, C++ and Python.
- **Parallel and High-Performance Languages:** Proficient in MPI, OpenMP, numba, dask, etc.
- **Programming for performance:** Extensive experience using debugging tools (DDT, Totalview, GDB and valgrind). Experience using parallel profiling tools(ARM/Forge, TAU, HPCtoolkit, Intel Vtune Amplifier, Intel Advisor, gprof, etc).
- **Software Skills:** *Quantum Mechanics:* NWChem, BigDFT, CP2k, CPMD, Quantum Expresso, OpenMX, FHIaims, Orca, HyperChem, etc. *Molecular Dynamics:* LAMMPS, Thinker, libatoms/QUIP, etc. *Chemioinformatics:* OpenBabel, RDkit, etc. *Machine Learning:* scikit-learn, Tensorflow, GPflow, QUIP, pytorch, etc. *Version Control and Engineering:* Git, SVN, Autotools, Cmake, etc.
- **General Business Skills:** Proficient in presentation skills and writing organized and structured reports. Ample experience working in a team to meet deadlines. Enthusiast troubleshooter.

Memberships

- Associate Member, American Physical Society (2015–present)
- Associate Member, American Chemical Society (2011–present)
- Fellow, National Mexican Council for Science and Technology (2009–present)

Peer-reviewed publications

1. Bagusetty, A, E.J. Bylaska, Álvaro Vázquez–Mayagoitia, and J.R. Hammond. "Transitioning ab-initio molecular dynamics simulations towards exascale heterogeneous computing". In: *Parallel Computing* (2021). Submitted.
2. Demiroğlu, İlker, Yenal Karaaslan, Tuğbey Kocabaş, Murat Keceli, Álvaro Vazquez-Mayagoitia, and Cem Sevik. "High Accuracy Estimation of Thermal Expansion Coefficient of Graphene by Machine Learning Gaussian Approximation Potential". In: *JPCC* (2021). Nanotechnology.
3. Al-Haddad, Andre et al. "Ultrafast chemical shifts during electron and nuclear rearrangements". In: *Science* (2021). Under review.
4. Hoja, J, L Medrano Sandonas, Ernst B., R.A. DiStassio Jr., Álvaro Vázquez-Mayagoitia, and A. Tkatchenko. "Quantum mechanics-based exploration of the chemical space of small molecules: database QM7X". In: *Scientific Data* (2021). Accepted.
5. Jain, Apoorv, Jacqueline M. Cole, Álvaro Vázquez-Mayagoitia, and Michael G. Sternberg. "Modeling dark- and light-induced crystal structures and single-crystal optical absorption spectra of ruthenium-based complexes that undergo SO2-linkage photoisomerization". In: *JPCC* (2021). In review.
6. Jeremy, Álvaro Sivaraman Ganesh Vázquez-Mayagoitia, and Michael G. Sternberg. "Uncertainty Informed Deep Transfer Learning of PFAS Toxicity". In: *TBD* (2021). Submitted.
7. Sivaraman, Ganesh, Leighanne Gallington, Anand Narayanan Krishnamoorthy, Marius Stan, Gabor Czany, Álvaro Vázquez-Mayagoitia, and Chris Benmore. "Experimentally driven automated machine-learned interatomic potential for a refractory oxide". In: *Physical Review Letters* (2021). Accepted.
8. Williams–Young, David B. et al. "Achieving Performance Portability in Gaussian Basis Set Density Functional Theory on Accelerator Based Architectures". In: *Parallel Computing* (2021). Submitted.

9. Aprá, Edo et al. "NWChem: Past, Present, and Future". In: *The Journal of Chemical Physics* 152 (2020), p. 184102.
10. Chen, Hao, Yun Gong, Álvaro Vázquez-Mayagoitia, and Jacqueline M. Cole. "Dye Aggregation, Photo-Structural Reorganization and Multiple Concurrent Dye $\cdots$ TiO_2 Binding Modes in Dye-sensitized Solar Cell Working Electrodes Containing Benzothiadiazole-Based Dye RK-1". In: *ACS Applied Energy Materials* 3.1 (2020), pp. 423–430.
11. Jackson, Nicholas E., Ganesh Sivaraman, Benjamin Sanchez-Lengeling, Álvaro Vázquez-Mayagoitia, Alan Aspurú-Guzik, Venkatram Vishwanath, and Juan J. de Pablo. "A diversified machine learning strategy for predicting, generating, and understanding molecular melting points". In: *IOP Machine Learning Science and Technology* (2020).
12. Rithwik, Tom, Timothy Rose, Bier Imanuel, Harriet O'Brien, Álvaro Vázquez-Mayagoitia, and Noa Marom. "Genarris 2.0: A random structure generator for molecular crystals". In: *Computer Physics Communications* (2020), p. 107170.
13. Sedenho, Graziela C., Diana De Porcellinis, Yan Jing, Emily Kerr, et al. "Effect of Molecular Structure of Quinones and Carbon Electrode Surfaces on the Interfacial Electron Transfer Process". In: *ACS Applied Energy Materials* 3.2 (2020), pp. 1933–1943. DOI: 10.1021/acsaem.9b02357.
14. Sivaraman, Ganesh, Gabor Czany, Chris Benmore, and Álvaro Vázquez-Mayagoitia. "Machine-Learned Inter-Atomic Potentials by Active Learning: Amorphous and Liquid Hafnium Dioxide". In: *NPJ Computational Materials* (2020). Accepted, https://arxiv.org/abs/1910.10254.
15. Sivaraman, Ganesh, Álvaro Vázquez-Mayagoitia, Venkatram Vishwanath, and Jacqueline M. Cole. "Chemical Cartography of Organic Dyes: Classification, Clustering and Low Dimensional Analysis of their Optical Absorption Properties". In: *JInfMol* (2020). In preparation.
16. Tom, Rithwik, Timothy Rose, Imanuel Bier, Harriet O'Brien, Álvaro Vazquez-Mayagoitia, and Noa Marom. "Genarris 2.0: A Random structure generator for molecular crystals". In: *Computer Physics Communications* 250 (2020). In press, p. 107170. DOI: https://doi.org/10.1016/j.cpc.2020.107170.
17. Yu, Victor Wen-zhe et al. "ELSI 2.0: An Open Infrastructure for Electronic Structure Solvers". In: *Computer Physics Communications* (2020). Under review, https://arxiv.org/abs/1912.13403.
18. Beard, Edward J., Ganesh Sivaraman, Álvaro Vázquez-Mayagoitia, and Jacqueline M. Cole. "Big data correlation of molar extinction coefficient with oscillator strength". In: *JCC* (2019). In preparation.
19. Beard, Edward J., Ganesh Sivarman, Álvaro Vázquez-Mayagoitia, Venkatram Vishwanath, and Jacqueline M. Cole. "Comparative dataset of experimental and computational attributes of UV/Vis absorption spectra". In: *Scientific Data* 307 (2019).
20. Cooper, Christopher B. et al. "Design to Device Approach Affords Panchromatic Co–sensitized Solar Cells". In: *Advanced Energy Materials, Wiley* (2019). In press https://doi.org/10.1002/aenm.201802820, Featured in cover issue.
21. Cruz, J. César, Raymundo Hernández-Esparza, Álvaro Vázquez-Mayagoitia, Rubicelia Vargas, and Jorge Garza. "Implementation of the Molecular Electrostatic Potential over Graphics Processing Units". In: *Journal of Chemical Information and Modeling* 59.7 (2019), pp. 3120–3127.
22. Ratcliff, Laura E., W. Scott Thornton, Álvaro Vázquez Mayagoitia, and Nichols A. Romero. "Combining Pseudopotential and All Electron Density Functional Theory for the Efficient Calculation of Core Spectra Using a Multiresolution Approach". In: *The Journal of Physical Chemistry A* 123.20 (2019), pp. 4465–4474.

23. Sedenho, Graziela C., Diana De Porcellinis, Yan Jing, Luis Martin Kerr Emily Mejia-Mendoza, et al. "How the molecular structure of quinones and carbon surface drive the interfacial electron transfer". In: *Nature Chemistry* (2019). Submitted.
24. Soriano-Agueda, Luis, Álvaro Vazquez-Mayagoitia, and Alberto Vela. "Spin-crossover with single determinant calculations of metal complexes and a comparison among CCSD, DFT and HF-DFT," in: *To be submitted* (2019).
25. Cruz-León, Sergio, Alvaro Vázquez-Mayagoitia, Simone Melchionna, Nadine Schwierz, and Maria Fyta. "Coarse-Grained Double-Stranded RNA Model from Quantum-Mechanical Calculations". In: *The Journal of Physical Chemistry B* 122.32 (2018), pp. 7915–7928.
26. Curtis, Farren, Xiayue Li, Álvaro Vázquez-Mayagoitia, Saswata Bhattacharya, Luca M. Ghiringhelli, and Noa Marom. "GAtor: A First-Principles Genetic Algorithm for Molecular Crystal Structure Prediction". In: *Journal of Chemical Theory and Computation* 14.4 (2018), pp. 2246–2264.
27. Ghadar, Yasaman, Álvaro Vazquez-Mayagoitia, Leighanne Gallington, John Low, Marius Stan, and Chris Benmore. "Determining the Structural Properties of HfO2 Utilizing Reactive Force Fields". In: *In preparation* (2018).
28. Hernadez, Raymundo, Álvaro Vázquez-Mayagoitia, Jorge Garza, and Rubicelia Vargas. "GPUs as boosters to analyze quantum chemistry fields". In: *International Journal of Quantum Chemistry* 112 (2 2018). https://doi.org/10.1002/qua.25671, Featured in cover issue, e25671.
29. Keceli, Murat et al. "Massively Parallel Spectrum Slicing Eigensolver for Ab Initio Calculations". In: *Journal of Computational Chemistry* 39.22 (2018), pp. 1806–1814.
30. Li, Xiayue et al. "Genarris: Random generation of molecular crystal structures and fast screening with a Harris approximation". In: *The Journal of Chemical Physics* 148.24 (2018), p. 241701.
31. Liu, Chi et al. "Tunable Semiconductors: Control over Carrier States and Excitations in Layered Hybrid Organic-Inorganic Perovskites". In: *Physics Review Letters* 121 (14 2018), p. 146401.
32. Yu, Victor Wen-zhe et al. "ELSI: A unified software interface for Kohn–Sham electronic structure solvers". In: *Computer Physics Communications* 222 (2018), pp. 267–285.
33. Cole, Jacqueline M et al. "Discovery of S··· CN Intramolecular Bonding in a Thiophenylcyanoacrylate-Based Dye: Realizing Charge Transfer Pathways and Dye··· TiO2 Anchoring Characteristics for Dye-Sensitized Solar Cells". In: *ACS applied materials & interfaces* 9.31 (2017), pp. 25952–25961.
34. Gallington, Leighanne C et al. "The Structure of Liquid and Amorphous Hafnia". In: *Materials* 10.11 (2017), p. 1290.
35. García-Hernández, Erwin, Roberto Flores-Moreno, Álvaro Vázquez-Mayagoitia, Rubicelia Vargas, and Jorge Garza. "Initial stage of the degradation of three common neonicotinoids: theoretical prediction of charge transfer sites". In: *New Journal of Chemistry* 41.3 (2017), pp. 965–974.
36. Moonshiram, Dooshaye et al. "Elucidating light-induced charge accumulation in an artificial analogue of methane monooxygenase enzymes using time-resolved X-ray absorption spectroscopy". In: *Chemical Communications* 53.18 (2017), pp. 2725–2728.
37. Pelzer, Kenley M et al. "Molecular dynamics and charge transport in organic semiconductors: a classical approach to modeling electron transfer". In: *Chemical science* 8.4 (2017), pp. 2597–2609.
38. Harrison, R. et al. "MADNESS: A Multiresolution, Adaptive Numerical Environment for Scientific Simulation". In: *SIAM Journal on Scientific Computing* 38.5 (2016), S123–S142.
39. Reilly, Anthony M et al. "Report on the sixth blind test of organic crystal structure prediction methods". In: *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials* 72.4 (2016), pp. 439–459.

40. Sullivan, Raymond, Junteng Jia, Álvaro Vázquez-Mayagoitia, and Antonio Picón. "Normal Auger processes with ultrashort x-ray pulses in neon". In: *Physical Review A* 94.4 (2016), p. 043421.
41. Cortés-Santiago, Avelino, Álvaro Vázquez-Mayagoitia, Jorge M del Campo, Luis A Soriano-Agueda, Rubicelia Vargas, and Jorge Garza. "Theoretical analysis of the S–P bond in a family of compounds that involve a P2S2 ring: role of the PBE0-1/5 exchange–correlation functional". In: *Computational and Theoretical Chemistry* 1062 (2015), pp. 36–43.
42. Beste, Ariana, Álvaro Vázquez-Mayagoitia, and J Vincent Ortiz. "Direct ΔMBPT (2) method for ionization potentials, electron affinities, and excitation energies using fractional occupation numbers". In: *The Journal of chemical physics* 138.7 (2013), p. 074101.
43. Montavon, Grégoire et al. "Machine learning of molecular electronic properties in chemical compound space". In: *New Journal of Physics* 15.9 (2013), p. 095003.
44. Willand, Alex et al. "Norm-conserving pseudopotentials with chemical accuracy compared to all-electron calculations". In: *The Journal of chemical physics* 138.10 (2013), p. 104109.
45. Burns, Lori A, Álvaro Vázquez- Mayagoitia, Bobby G Sumpter, and C David Sherrill. "Density-functional approaches to noncovalent interactions: a comparison of dispersion corrections (DFT-D), exchange-hole dipole moment (XDM) theory, and specialized functionals". In: *The Journal of chemical physics* 134.8 (2011), p. 084107.
46. Vázquez-Mayagoitia, Álvaro, Scott R Horton, Bobby G Sumpter, Jiři Šponer, Judit E Šponer, and Miguel Fuentes-Cabrera. "On the stabilization of ribose by silicate minerals". In: *Astrobiology* 11.2 (2011), pp. 115–121.
47. Šponer, Judit E et al. "Theoretical Studies on the Intermolecular Interactions of Potentially Primordial Base-Pair Analogues". In: *Chemistry-A European Journal* 16.10 (2010), pp. 3057–3065.
48. Vázquez-Mayagoitia, Álvaro, Jorge Garza, Rubicelia Vargas, Carlos Frontana, Martın Gómez, Ignacio González, and José L Gázquez. "Simple charge transfer model for one electron oxidation and reduction processes: Describing reactive sites in benzocarbazolediones and gallates". In: *Journal of Molecular Structure: THEOCHEM* 943.1-3 (2010), pp. 59–64.
49. Vazquez-Mayagoitia, Álvaro, C David Sherrill, Edoardo Apra, and Bobby G Sumpter. "An assessment of density functional methods for potential energy curves of nonbonded interactions: the XYG3 and B97-D approximations". In: *Journal of chemical theory and computation* 6.3 (2010), pp. 727–734.
50. Harrison, Robert J, Edoardo Apra, William Allison Shelton Jr, Vinod Tipparaju, and Álvaro Vazquez-Mayagoitia. "Computational Chemistry at the Petascale: Are We There Yet?" In: (2009).
51. Vázquez-Mayagoitia, Álvaro, Oscar Huertas, Giorgia Brancolini, et al. "Ab initio Study of the Structural, Tautomeric, Pairing, and Electronic Properties of Seleno-Derivatives of Thymine". In: *The Journal of Physical Chemistry B* 113.43 (2009), pp. 14465–14472.
52. Vázquez-Mayagoitia, Álvaro, Oscar Huertas, Miguel A. Fuentes-Cabrera, Modesto Orozco, Javier Luque, and Bobby G Sumpter. "Ab initio Study of Naptho-Homologated DNA Bases". In: *Journal of Physical Chemistry B* 112.7 (2008).
53. Sumpter, Bobby G, Vincent Meunier, Álvaro Vázquez-Mayagoitia, and Ronald K Castellano. "Investigation of the nanoscale self-assembly of donor-σ-acceptor molecules". In: *International Journal of Quantum Chemistry* 107.12 (2007), pp. 2233–2242.
54. Frontana, Carlos, Álvaro Vázquez-Mayagoitia, Jorge Garza, Rubicelia Vargas, and Ignacio González. "Substituent effect on a family of quinones in aprotic solvents: an experimental and theoretical approach". In: *The Journal of Physical Chemistry A* 110.30 (2006), pp. 9411–9419.

55. Vázquez-Mayagoitia, Álvaro, Rubicelia Vargas, Jeffrey A Nichols, Patricio Fuentealba, and Jorge Garza. "Relationship between singlet–triplet excitation energies and the Kohn–Sham orbitals obtained with potentials that exhibit a wrong asymptotic behavior". In: *Chemical physics letters* 419.1-3 (2006), pp. 207–212.

Technical reports

1. Blum, Volker et al. *Electronic Structure-Based Discovery of Hybrid Photovoltaic Materials on Next-Generation HPC Platforms: Theta Early Science Program Technical Report*. Argonne National Laboratory (ANL), 2017.
2. Harrison, Robert J., Álvaro Vazquez-Mayagoitia, and Jeff R. Hammond. *Accurate Numerical Simulations Of Chemical Phenomena Involved in Energy Production and Storage with MADNESS and MPQC: ALCF-2 Early Science Program Technical Report*. Argonne National Laboratory (ANL), 2013.

Book Chapters

1. Fahey, Mark et al. "Theta and Mira". In: *Contemporary High Performance Computing*. CRC Press, Inc., 2018.
2. Vázquez–Mayagoitia, Álvaro, W Scott Thornton, Jeff R. Hammond, and Robert J. Harrison. "Quantum Chemistry Methods with Multiwavelet Bases on Massive Parallel Computers". In: *Annual Reports in Computational Chemistry*. Vol. 10. Elsevier, 2014, pp. 3–24.
3. Huang, Jingsong et al. "Advancing understanding and design of functional materials through theoretical and computational chemical physics". In: *Practical Aspects of Computational Chemistry II*. Springer Netherlands, 2012, pp. 209–278.

*Copies of draft publications : to be submitted, in review, and in press, are available upon request.