Dr. Fernando D. Vila

CONTACT INFORMATION

Staff Scientist
University of Washington
Department of Physics
Box 351560, Room B430
Seattle, WA 98195-1560, USA

Work: +1-206-543-9697
Fax: +1-206-685-0635
E-mail: fdv@uw.edu
WWW: staff.washington.edu/fdv

RESEARCH INTERESTS

Theoretical condensed matter physics, chemistry and spectroscopy: Excited states, optical and X-ray spectroscopy, chemical reactivity, catalysis at the nanoscale, nuclear and electronic real-time dynamics, intermolecular interactions, scientific software development.

CURRENT ACADEMIC APPOINTMENT

Staff Scientist Jan 2005 – Present

Dept. of Physics, Univ. of Washington

- Supervisor: Prof. John J. Rehr
- Lead and pursue a wide variety of lines of research. Engage in multidisciplinary research in the areas of materials science, condensed matter physics, theoretical chemistry and spectroscopy.
- Lead, participate and manage the development of new scientific software. Co-developer of the widely-used real-space multiple scattering code FEFF. Original developer of SC2VP/SC2IT, a scientific cloud computing platform for materials science, condensed matter physics and computational chemistry.
- Lead and participate in the writing of successful funding proposals. Wrote and coordinated the submission of a successful NSF proposal to develop Scientific Cloud Computing Software. Led yearly successful allocation requests for supercomputer time.
- Manage graduate and undergraduate research. Mentored undergraduate students in the REU program.

PREVIOUS ACADEMIC APPOINTMENTS

Postdoctoral Research Associate Aug 2003 – Dec 2005

Dept. of Physics, Univ. of Washington

- Supervisor: Prof. John J. Rehr
- Affiliations: Center on Materials and Devices for Information Technology Research
- Co-developer of RT-SIESTA, a real-time time-dependent density functional theory code for the realistic simulation of the interaction between matter and radiation.
- Studied the linear and non-linear optical response of organic materials of interest in information technology

Postdoctoral Research Associate Jan 2001 – Aug 2003

Dept. of Chemistry, Univ. of Washington

- Supervisor: Prof. Hannes Jónsson
- Worked in the development of a transferable, single-center interaction potential for water

Research and Teaching Assistant Jan 1996 – Aug 1998

Dept. of Chemistry, Univ. of Pittsburgh

- Supervisor: Prof. Kenneth Jordan
- Studied dipole-bound anions, weakly interacting and hydrogen-bonded sytems
- Studied the low-lying excited states of organic molecules with complex electronic structure

Profesor (Grado 1) Mar 1992 – Dec 1995

Facultad de Química, Univ. de la República

- Supervisor: Prof. Oscar N. Ventura
- Studied the excited states of the water monomer and dimer
- Studied the sintering of zinc-oxide in the presence of different gases

EDUCATION

Univ. of Pittsburgh, Pittsburgh, PA

Ph.D., Chemistry, Dec 2000

- Thesis Topic: *Electron-Molecule Interactions*
- Advisor: Prof. Kenneth Jordan
- Area of Study: Theoretical Chemistry

Univ. de la República, Montevideo, Uruguay

M.Sc., Chemistry, Dec 1995

- Thesis Topic: *Theoretical study of the low-lying and Rydberg excited states in the water monomer and dimer*
- Advisor: Prof. Oscar N. Ventura
- Area of Study: Quantum Chemistry

B. Sc., Chemistry, Dec 1991

- Area of Study: Chemical Engineering

EXPERTISE

Theoretical chemistry:

- Chemical reactivity
- Intermolecular interactions and hydrogen bonding
- Post-Hartree-Fock methods (MPn, CC, MRCI, CASSCF)

Theoretical spectroscopy:

- Infrared, UV-Vis and X-ray spectroscopies
- Excited states, linear and non-linear optical properties
- Nuclear and electron real-time dynamics

Theoretical condensed matter physics:

- Density Functional Theory, Molecular Dynamics
- Energy-related materials and catalysis at the nanoscale

Scientific software and programming:

- Molecular codes: Gaussian, StoBe, and NWChem
- Condensed matter codes: FEFF, VASP, ABINIT, and Siesta
- High-performance scientific computing and programming
- Parallel and distributed computing

SUBMITTED JOURNAL PUBLICATIONS

[1] F.D. Vila, J.J. Rehr, J.J. Kas, K. Kowalski and B. Peng , "Real-time coupled-cluster approach for the cumulant Green's function", *Submitted to Journal of Chemical Theory and Computation*.

REFEREED JOURNAL PUBLICATIONS

[1] S.K. Gill, J. Huang, J. Mausz, R. Gakhar, S. Roy, F.D. Vila, M. Topsakal, W.C. Phillips, B. Layne, S. Mahurin, and others, "Connections between the Speciation and Solubility of Ni (II) and Co (II) in Molten $ZnCl_2$", *J. Phys. Chem. B* **124** (2020) 1253.
doi:10.1021/acs.jpcb.0c00195 [URL]

[2] J.J. Rehr, F.D. Vila, J.J. Kas, N. Hirshberg, K. Kowalski, and B. Peng, "Equation of motion coupled-cluster cumulant approach for intrinsic losses in x-ray spectra", *J. Chem. Phys.* **152** (2020) 174113.
doi:10.1063/5.0004865 [URL]

[3] O. Travnikova, M. Patanen, J. Söderström, A. Lindblad, J. Kas, F. Vila, D. Céolin, C. Nicolas, T. Marchenko, G. Goldsztejn, and others, "Energy dependent relative cross sections in carbon 1s photoionization", *J. Phys. Conf. Ser.* **1412** (2020) 152050.
doi:10.1088/1742-6596/1412/15/152050 [URL]

[4] A.S. Asundi, A.S. Hoffman, P. Bothra, A. Boubnov, F.D. Vila, N. Yang, J.A. Singh, L. Zeng, J.A. Raiford, F. Abild-Pedersen, and others, "Understanding Structure–Property Relationships of MoO3-Promoted Rh Catalysts for Syngas Conversion to Alcohols", *J. Am. Chem. Soc.* **141** (2019) 19655.
doi:10.1021/jacs.9b07460 [URL]

[5] S.M. Story, F.D. Vila, J.J. Kas, K.B. Raniga, C.D. Pemmaraju, and J.J. Rehr, "Corvus: a framework for interfacing scientific software for spectroscopic and materials science applications", *J. Synchrotron Radiat.* **26** (2019) .
doi:10.1107/S1600577519007495 [URL]

[6] O. Travnikova, M. Patanen, J. Soderstrom, A. Lindblad, J.J. Kas, F.D. Vila, D. Céolin, T. Marchenko, G. Goldsztejn, R. Guillemin, and others, "Energy-Dependent Relative Cross Sections in Carbon 1s Photoionization: Separation of Direct Shake and Inelastic Scattering Effects in Single Molecules", *J. Phys. Chem. A* **123** (2019) 7619.
doi:10.1021/acs.jpca.9b05063 [URL]

[7] C.D. Pemmaraju, F.D. Vila, J.J. Kas, S.A. Sato, J.J. Rehr, K. Yabana, and D. Prendergast, "Velocity-gauge real-time TDDFT within a numerical atomic orbital basis set", *Comput. Phys. Commun.* **226** (2018) 30.
doi:10.1016/j.cpc.2018.01.013 [URL]

[8] F.D. Vila, S.T. Hayashi, and J.J. Rehr, "Efficient calculation of the negative thermal expansion in ZrW_2O_8", *Front. Chem.* **6** (2018) 296.
doi:10.3389/fchem.2018.00296 [URL]

[9] F.D. Vila, J.W. Spencer, J.J. Kas, J.J. Rehr, and F. Bridges, "Extended X-Ray Absorption Fine Structure of ZrW_2O_8: Theory vs. Experiment", *Front. Chem.* **6** (2018) 356.
doi:10.3389/fchem.2018.00356 [URL]

[10] S. Vimolchalao, W.H. Liang, F.D. Vila, J.J. Kas, F. Farges, and J.J. Rehr, "Bethe-Salpeter Equation calculations of nitrogen-vacancy defects in diamond", *J. Phys. Chem. Solids* **122** (2018) 87.
doi:10.1016/j.jpcs.2018.06.006 [URL]

[11] C. Zheng, K. Mathew, C. Chen, Y. Chen, H. Tang, A. Dozier, J.J. Kas, F.D. Vila, J.J. Rehr, L.F. Piper, and others, "Automated generation and ensemble-learned matching of X-ray absorption spectra", *npj Comput. Mater.* **4** (2018) 12.
doi:10.1038/s41524-018-0067-x [URL]

[12] S.R. Bare, F.D. Vila, M.E. Charochak, S. Prabhakar, W.J. Bradley, C. Jaye, D.A. Fischer, S.T. Hayashi, S.A. Bradley, and J.J. Rehr, "Characterization of Coke on a Pt-Re/γ-Al_2O_3 Re-Forming Catalyst: Experimental and Theoretical Study", *ACS Catal.* **7** (2017) 1452.
doi:10.1021/acscatal.6b02785 [URL]

[13] F. Fossard, G. Hug, K. Gilmore, J.J. Kas, J.J. Rehr, F.D. Vila, and E.L. Shirley, "Quantitative first-principles calculations of valence and core excitation spectra of solid C_{60}", *Phys. Rev. B* **95** (2017) 115112.
doi:10.1103/PhysRevB.95.115112 [URL]

[14] F.D. Vila, J.J. Rehr, R.G. Nuzzo, and A.I. Frenkel, "Anomalous Structural Disorder in Supported Pt Nanoparticles", *J. Phys. Chem. Lett.* **8** (2017) 3284. doi:10.1021/acs.jpclett.7b01446 [URL]

[15] E. Klevak, F.D. Vila, J.J. Kas, J.J. Rehr, and G.T. Seidler, "Finite-temperature calculations of the Compton profile of Be, Li, and Si", *Phys. Rev. B* **94** (2016) 214201. doi:10.1103/PhysRevB.94.214201 [URL]

[16] F.D. Vila, S.T. Hayashi, J.M. Moore, and J.J. Rehr, "Molecular Dynamics Simulations of Supported Pt Nanoparticles with a Hybrid Sutton-Chen Potential", *J. Phys. Chem. C* **120** (2016) 14883. doi:10.1021/acs.jpcc.6b03074 [URL]

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[18] A. Elsen, U. Jung, F.D. Vila, Y. Li, O.V. Safonova, R. Thomas, M. Tromp, J.J. Rehr, R.G. Nuzzo, and A.I. Frenkel, "Intracluster Atomic and Electronic Structural Heterogeneities in Supported Nanoscale Metal Catalysts", *J. Phys. Chem. C* **119** (2015) 25615. doi:10.1021/acs.jpcc.5b08267 [URL]

[19] K. Gilmore, J. Vinson, E.L. Shirley, D. Prendergast, C.D. Pemmaraju, J.J. Kas, F.D. Vila, and J.J. Rehr, "Efficient implementation of core-excitation Bethe-Salpeter equation calculations", *Comput. Phys. Commun.* **197** (2015) 109. doi:10.1016/j.cpc.2015.08.014 [URL]

[20] J.J. Kas, F.D. Vila, J.J. Rehr, and S.A. Chambers, "Real-time cumulant approach for charge-transfer satellites in x-ray photoemission spectra", *Phys. Rev. B* **91** (2015) 121112. doi:10.1103/PhysRevB.91.121112 [URL]

[21] A.I. Frenkel, M.W. Cason, A. Elsen, U. Jung, M.W. Small, R.G. Nuzzo, F.D. Vila, J.J. Rehr, E.A. Stach, and J.C. Yang, "Critical review: Effects of complex interactions on structure and dynamics of supported metal catalysts", *J. Vac. Sci. Technol., A* **32** (2014) 020801. doi:10.1116/1.4820493 [URL]

[22] L. He, F. Liu, G. Hautier, M.J.T. Oliveira, M.A.L. Marques, F.D. Vila, J.J. Rehr, G.-M. Rignanese, and A. Zhou, "Accuracy of generalized gradient approximation functionals for density-functional perturbation theory calculations", *Phys. Rev. B* **89** (2014) 064305. doi:10.1103/PhysRevB.89.064305 [URL]

[23] J.J. Rehr, and F.D. Vila, "Dynamic structural disorder in supported nanoscale catalysts", *J. Chem. Phys.* **140** (2014) 134701. doi:10.1063/1.4869178 [URL]

[24] S.M. Story, J.J. Kas, F.D. Vila, M.J. Verstraete, and J.J. Rehr, "Cumulant expansion for phonon contributions to the electron spectral function", *Phys. Rev. B* **90** (2014) 195135. doi:10.1103/PhysRevB.90.195135 [URL]

[25] T.X. Carroll, M.G. Zahl, K.J. Børve, L.J. Sæthre, P. Decleva, A. Ponzi, J.J. Kas, F.D. Vila, J.J. Rehr, and T.D. Thomas, "Intensity oscillations in the carbon 1s ionization cross sections of 2-butyne", *J. Chem. Phys.* **138** (2013) 234310. doi:10.1063/1.4810870 [URL]

[26] N. Mårtensson, J. Söderström, S. Svensson, O. Travnikova, M. Patanen, C. Miron, L.J. Sæthre, K.J. Børve, T.D. Thomas, J.J. Kas, F.D. Vila, and J.J. Rehr, "On the relation between X-ray Photoelectron Spectroscopy and XAFS", *J. Phys. Conf. Ser.* **430** (2013) 012131. doi:10.1088/1742-6596/430/1/012131 [URL]

[27] F.D. Vila, J.J. Rehr, S.D. Kelly, and S.R. Bare, "Operando Effects on the Structure and Dynamics of Pt_nSn_m/γ-Al_2O_3 from Ab Initio Molecular Dynamics and X-ray Absorption Spectra", *J. Phys. Chem. C* **117** (2013) 12446. doi:10.1021/jp403931z [URL]

[28] K.T. Wikfeldt, E.R. Batista, F.D. Vila, and H. Jonsson, "A transferable H_2O interaction potential based on a single center multipole expansion: SCME", *Phys. Chem. Chem. Phys.* **15** (2013) 16542. doi:10.1039/C3CP52097H [URL]

[29] M.A. Brown, F.D. Vila, M. Sterrer, S. Thürmer, B. Winter, M. Ammann, J.J. Rehr, and J.A. van Bokhoven, "Electronic Structures of Formic Acid (HCOOH) and Formate ($HCOO^-$) in Aqueous Solutions", *J. Phys. Chem. Lett.* **3** (2012) 1754. doi:10.1021/jz300510r [URL]

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[31] K. Jorissen, F.D. Vila, and J.J. Rehr, "A high performance scientific cloud computing environment for materials simulations", *Comput. Phys. Commun.* **183** (2012) 1911. doi:10.1016/j.cpc.2012.04.010 [URL]

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[33] J. Söderström, N. Mårtensson, O. Travnikova, M. Patanen, C. Miron, L.J. Sæthre, K.J. Børve, J.J. Rehr, J.J. Kas, F.D. Vila, T.D. Thomas, and S. Svensson, "Non-stoichiometric Intensities in Core Photoelectron Spectroscopy", *Phys. Rev. Lett.* **108** (2012) 193005. doi:10.1103/PhysRevLett.108.193005 [URL]

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[36] T. Ahmed, T. Das, J.J. Kas, H. Lin, B. Barbiellini, F.D. Vila, R.S. Markiewicz, A. Bansil, and J.J. Rehr, "X-ray absorption near-edge spectra of overdoped $La_{2-x}Sr_xCuO_4$ high-T_c superconductors", *Phys. Rev. B* **83** (2011) 115117. doi:10.1103/PhysRevB.83.115117 [URL]

[37] S.R. Bare, S.D. Kelly, F. D.Vila, E. Boldingh, E. Karapetrova, J. Kas, G.E. Mickelson, F.S. Modica, N. Yang, and J.J. Rehr, "Experimental (XAS, STEM, TPR, and XPS) and Theoretical (DFT) Characterization of Supported Rhenium Catalysts", *J. Phys. Chem. C* **115** (2011) 5740.
doi:10.1021/jp1105218 [URL]

[38] F.D. Vila, T. Jach, W.T. Elam, J.J. Rehr, and J.D. Denlinger, "X-ray Emission Spectroscopy of Nitrogen-Rich Compounds", *J. Phys. Chem. A* **115** (2011) 3243.
doi:10.1021/jp108539v [URL]

[39] J.J. Rehr, J.J. Kas, F.D. Vila, M.P. Prange, and K. Jorissen, "Parameter-free calculations of X-ray spectra with FEFF9", *Phys. Chem. Chem. Phys.* **12** (2010) 5503.
doi:10.1039/B926434E [URL]

[40] J.J. Rehr, F.D. Vila, J.P. Gardner, L. Svec, and M. Prange, "Scientific Computing in the Cloud", *Computing in Science & Engineering* **12** (2010) 34.
doi:10.1109/MCSE.2010.70 [URL]

[41] G. Veronesi, C. Degli Esposti Boschi, L. Ferrari, G. Venturoli, F. Boscherini, F.D. Vila, and J.J. Rehr, "*Ab initio* analysis of the x-ray absorption spectrum of the myoglobin-carbon monoxide complex: Structure and vibrations", *Phys. Rev. B* **82** (2010) 020101.
doi:10.1103/PhysRevB.82.020101 [URL]

[42] F.D. Vila, D.A. Strubbe, Y. Takimoto, X. Andrade, A. Rubio, S.G. Louie, and J.J. Rehr, "Basis set effects on the hyperpolarizability of $CHCl_3$: Gaussian-type orbitals, numerical basis sets and real-space grids", *J. Chem. Phys.* **133** (2010) 034111.
doi:10.1063/1.3457362 [URL]

[43] T.T. Fister, K.P. Nagle, F.D. Vila, G.T. Seidler, C. Hamner, J.O. Cross, and J.J. Rehr, "Intermediate-range order in water ices: Nonresonant inelastic x-ray scattering measurements and real-space full multiple scattering calculations", *Phys. Rev. B* **79** (2009) 174117.
doi:10.1103/PhysRevB.79.174117 [URL]

[44] J.J. Rehr, J.J. Kas, M.P. Prange, A.P. Sorini, Y. Takimoto, and F.D. Vila, "Ab initio theory and calculations of X-ray spectra", *C. R. Phys.* **10** (2009) 548.
doi:10.1016/j.crhy.2008.08.004 [URL]

[45] T.T. Fister, G.T. Seidler, E.L. Shirley, F.D. Vila, J.J. Rehr, K.P. Nagle, J.C. Linehan, and J.O. Cross, "The local electronic structure of α-Li_3N", *J. Chem. Phys.* **129** (2008) 044702.
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[46] T.T. Fister, F.D. Vila, G.T. Seidler, L. Svec, J.C. Linehan, and J.O. Cross, "Local Electronic Structure of Dicarba-closo-dodecarboranes $C_2B_{10}H_{12}$", *J. Am. Chem. Soc.* **130** (2008) 925.
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[47] H.M. Lawler, J.J. Rehr, F.D. Vila, S.D. Dalosto, E.L. Shirley, and Z.H. Levine, "Optical to UV spectra and birefringence of SiO_2 and TiO_2: First-principles calculations with excitonic effects", *Phys. Rev. B* **78** (2008) 205108.
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[48] F.D. Vila, J.J. Rehr, J.J. Kas, R.G. Nuzzo, and A.I. Frenkel, "Dynamic structure in supported Pt nanoclusters: Real-time density functional theory and x-ray

spectroscopy simulations", *Phys. Rev. B* **78** (2008) 121404. doi:10.1103/PhysRevB.78.121404 [URL]

[49] C.M. Isborn, A. Leclercq, F.D. Vila, L.R. Dalton, J.L. Brédas, B.E. Eichinger, and B.H. Robinson, "Comparison of Static First Hyperpolarizabilities Calculated with Various Quantum Mechanical Methods", *J. Phys. Chem. A* **111** (2007) 1319. doi:10.1021/jp064096g [URL]

[50] Y. Takimoto, F.D. Vila, and J.J. Rehr, "Real-time time-dependent density functional theory approach for frequency-dependent nonlinear optical response in photonic molecules", *J. Chem. Phys.* **127** (2007) 154114. doi:10.1063/1.2790014 [URL]

[51] F.D. Vila, J.J. Rehr, H.H. Rossner, and H.J. Krappe, "Theoretical x-ray absorption Debye-Waller factors", *Phys. Rev. B* **76** (2007) 014301. doi:10.1103/PhysRevB.76.014301 [URL]

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[55] E.P. Clifford, P.G. Wenthold, W. Carl Lineberger, G. Barney Ellison, C. X. Wang, J. J. Grabowski, F.D. Vila, and K. D. Jordan, "Properties of tetramethyleneethane (TME) as revealed by ion chemistry and ion photoelectron spectroscopy", *J. Chem. Soc., Perkin Trans. 2* (1998) 1015. doi:10.1039/A707322D [URL]

[56] J.M. Pedulla, F.D. Vila, and K.D. Jordan, "Binding energy of the ring form of $(H_2O)_6$: Comparison of the predictions of conventional and localized-orbital MP2 calculations", *J. Chem. Phys.* **105** (1996) 11091. doi:10.1063/1.472910 [URL]

[57] F.D. Vila, O.N. Ventura, J.A. Varela, and E. Longo, "An AM1 semiempirical study of the mechanism of sintering for ZnO in the presence of water and carbon dioxide", *J. Mol. Struct. THEOCHEM* **305** (1994) 175. doi:10.1016/0166-1280(94)80152-5 [URL]

Conference Publications

[1] A. Dozier, K. Persson, S. Ping Ong, K. Mathew, C. Zheng, C. Chen, J. Kas, F. Vila, and J. Rehr, "Creation of an XAS and EELS Spectroscopy Resource within the Materials Project using FEFF9", *Microsc. Microanal.* **23** (2017) 208. doi:10.1017/S1431927617001726 [URL]

[2] G.J. Havrilla, K. Mcintosh, M. Croce, R. Huber, D. Podlesak, M. Rabin, F. Vila, M. Carpenter, and R. Cantor, "Carbon Bonding Determination with XES Using a TES Microcalorimeter Detector", *Microsc. Microanal.* **23** (2017) 1060. doi:10.1017/S1431927617005967 [URL]

[3] J.J. Rehr, J.J. Kas, M.P. Prange, A.P. Sorini, L.W. Campbell, and F.D. Vila, "Inelastic Losses and Multi-Electron Excitations in X-Ray Spectra", *AIP Conference*

Proceedings **882** (2007) 85.
doi:10.1063/1.2644437 [URL]

[4] N. Yang, G.E. Mickelson, N. Greenlay, S.D. Kelly, F.D. Vila, J. Kas, J.J. Rehr, and S.R. Bare, "Size and Shape of Rhenium Nanoparticles", *AIP Conference Proceedings* **882** (2007) 591.
doi:10.1063/1.2644602 [URL]

BOOK CHAPTERS

[1] J.J. Rehr, J.J. Kas, F.D. Vila and M. Newville "Theory and Analysis of XAFS." In *XAFS Techniques for Catalysts, Nanomaterials, and Surfaces,* edited by Y. Iwasawa, K. Asakura, M. Tada, pages 13-50. Springer, Cham, 2017.

OTHER PUBLICATIONS

[1] K. Jorissen, J. J. Rehr, J. Kas and F. D. Vila, "New Developments in FEFF: FEFF9 and JFEFF", *IXAS Research Review* 7, (2012).

INVITED TALKS

[1] "Real-time and finite temperature Green's function approaches for excited states, response functions, and thermodynamics", *Recent Advances in DFT & TDDFT: Theory & Simulations, 256rd American Chemical Society National Meeting*, Aug 19-23, 2018, Boston, MA. [PDF]

[2] "Exploring the anomalous behavior of metal nanocatalysts with finite temperature AIMD and x-ray spectra", *Advances in X-Ray Techniques for Catalyst Characterization: Theory and Beyond, 253rd American Chemical Society National Meeting*, Apr 2-6, 2017, San Francisco, CA. [PDF]

[3] "Theory and Parameter Free Calculations of EELS and X-ray Spectra", *Combining Simulation, Experiment, and Data Science for Materials Characterization and Design, Microscopy and Microanalysis*, Jul 24-28, 2016, Columbus, OH. [PDF]

[4] "Advances in electronic structure, vibrations and disorder in FEFF", *Seminar and Demonstration at the Brazilian Synchrotron Light Source*, Apr 13-14, 2015, Campinhas, Brazil. [PDF]

[5] "RT-SIESTA: Real-time linear and non-linear response for optical and core spectroscopies, Vanderbilt University", *Quantum Dynamics Research Meeting*, Mar 10, 2014, Nashville, TN. [PDF]

[6] "Dynamic structure of supported Pt and Pt-Sn nanocatalysts: Real-time DFT/MD and X-ray Spectroscopy simulations", *UOP Colloquium, UOP, A Honeywell Company*, May 8, 2013, Des Plaines, IL. [PDF]

[7] "Estructura dinámica en nanopartículas de Pt y Pt-Sn", *DETEMA Colloquium, Univ. de la República*, Aug 26, 2013, Montevideo, Uruguay. [PDF]

[8] "Cloud Computing Clusters for Scientific Research", *NSF PI Meeting: The Science of the Cloud*, Mar 17-18, 2011, Arlington, VA. [PDF]

[9] "Fast and Ultrafast Phenomena", *Computational Scattering Science Workshop, ANL*, Jul 8, 2010, Lemont, IL. [PDF]

[10] "First Principles Structure, Dynamics and X-Ray Spectroscopy of Complex Systems", *Molecular Foundry Colloquium, LBNL*, Jun 1, 2009, Berkeley, CA. [PDF]

[11] "Real-Space and Real-Time Approaches for Energy-Related Materials", *Workshop on Advanced Materials for Energy Applications, ALS*, Oct 15-17, 2009, Berkeley, CA. [PDF]

[12] "Scientific Cloud Computing", *Envisioning XD: Cloud Computing Workshop, ANL*, Sep 29-30, 2009, Lemont, IL. [PDF]

CONTRIBUTED TALKS

[1] "Real-time EOM-CCS Green's function method for the core spectral functions", *American Physical Society (March Meeting, Cancelled)*, Mar 2-6, 2020, Denver, CO. [PDF]

[2] "Efficient Implementation of RT-TDDFT on Siesta 4.0", *American Physical Society (March Meeting)*, Mar 4-8, 2019, Boston, MA. [PDF]

[3] "Dynamic anomalies in the nanoscale structure and disorder of supported metal nanoparticles", *The 17th International Conference on X-ray Absorption Fine Structure (XAFS17)*, Jul 22-27, 2018, Krakow, Poland. [PDF]

[4] "Dynamic and static disorder in supported Pt nanoparticles: when static is not static", *American Physical Society (March Meeting)*, Mar 13-17, 2017, New Orleans, LA. [PDF]

[5] "Parallel calculations of vibrational properties in complex materials: negative thermal expansion and elastic inhomogeneity", *American Physical Society (March Meeting)*, Mar 14-18, 2016, Baltimore, MD. [PDF]

[6] "Structural and charge inhomogeneity in supported Pt clusters", *American Physical Society (March Meeting)*, Mar 2-6, 2015, San Antonio, TX. [PDF]

[7] "Dynamic structural disorder and reactivity in supported metal nanocatalysts", *The 16th International Conference on X-ray Absorption Fine Structure (XAFS16)*, Aug 23-28, 2015, Karlsruhe, Germany. [PDF]

[8] "Nanosecond Dynamics in Pt Nanoparticles", *American Physical Society (March Meeting)*, Mar 3-7, 2014, Denver, CO. [PDF]

[9] "Dynamic Structural Disorder in Supported Nanoparticles", *American Physical Society (March Meeting)*, Mar 18-22, 2013, Baltimore, MD. [PDF]

[10] "Real-time time-correlation approach for x-ray absorption and emission spectra", *American Physical Society (March Meeting)*, Feb 27-Mar 2, 2012, Boston, MA. [PDF]

[11] "Thermal and composition effects on the structure, dynamics, and reactivity of PtSn bimetallic nanoparticles on γ-Al_2O_3", *The 15th International Conference on X-ray Absorption Fine Structure (XAFS15)*, Jul 22-28, 2012, Beijing, China. [PDF]

[12] "Structure and dynamics of PtSn/γAl_2O_3", *American Physical Society (March Meeting)*, Mar 21-25, 2011, Dallas, TX. [PDF]

[13] "RT-TDDFT Simulations of NLO-Polymers with Tunable Energy Levels", *American Physical Society (March Meeting)*, Mar 15-19, 2010, Portland, OR. [PDF]

[14] "RT-TDDFT simulation of the optical properties of a model organic photovoltaic device", *American Physical Society (March Meeting)*, Mar 16-20, 2009, Pittsburgh, PA. [PDF]

[15] "Dynamic structure in Pt nanoclusters on gamma-alumina", *American Physical Society (March Meeting)*, Mar 10-14, 2008, New Orleans, LA. [PDF]

[16] "Ab Initio XAS Debye-Waller Factors Beyond the Harmonic Approximation", *American Physical Society (March Meeting)*, Mar 5-9, 2007, Denver, CO. [PDF]

[17] "Ab initio X-Ray Absorption Fine Structure Cumulants", *American Physical Society (March Meeting)*, Mar 13-17, 2006, Baltimore, MD. [PDF]

[18] "Theoretical Calculations of Nonlinear Optical Response", *American Physical Society (March Meeting)*, Mar 21-25, 2005, Los Angeles, CA. [PDF]

[19] "Molecular Properties of the Ice Ih Basal Surface: An Application of the SCME Water Interaction Potential", *American Chemical Society Northwest Regional Meeting*, May 30-31, 2003, Portland, OR. [PDF]

ACADEMIC SERVICE

2019 SSRL/LCLS Users' Meeting
"Developments & Challenges in X-ray Spectroscopies and Ultrafast Dynamics: Experiment and Theory" Organizer, SLAC National Lab. 2019.

Computational Scattering Science 2010
"Fast and Ultrafast Phenomena" Topic Leader, Argonne National Lab. 2010.

Envisioning XD: Cloud Computing
Invited consulter, Argonne National Lab. 2009.

STUDENT ADVISING & MENTORING

Scott T. Hayashi
Undergraduate student in Physics, Univ. of Washington. *Development of a model potential to simulate Pt nanoclusters on γ-Al_2O_3.* Primary advisor: Prof. J. J. Rehr. 2013 – Present.

Siri Vimolchalao
Undergraduate student in Physics, Univ. of Washington. *Simulation of the optical properties of diamond and TiO_2 using AI2NBSE and FEFF.* Primary advisor: Prof. J. J. Rehr. 2013 – Present.

Egor Klevak
Graduate student in Physics, Univ. of Washington. *Developments in the Theory of X-ray Absorption and Compton Scattering.* Primary advisor: Prof. J. J. Rehr. 2013 – 2016.

Shauna Story
Graduate student in Physics, Univ. of Washington. *Ab initio calculations of phonon properties and spectra in condensed matter.* Primary advisor: Prof. J. J. Rehr. 2013 – 2015.

Winnie Liang
REU student in Physics, Univ. of Washington. *Simulation of the optical response of colored diamods.* Primary advisor: Prof. J. J. Rehr. Jun – Aug 2014.

Jeffrey M. Moore
REU student in Physics, Univ. of Washington. *Development of a model potential to simulate Pt nanocluster on γ-Al_2O_3.* Primary advisor: Prof. J. J. Rehr. Jun – Aug 2013.

Viveca Lindahl
REU student in Physics, Univ. of Washington. *Development of a real-time method for the computation of EXAFS Debye-Waller factors based on ab initio molecular dynamics.* Primary advisor: Prof. J. J. Rehr. Jun – Aug 2010.

TEACHING EXPERIENCE

Brookhaven National Laboratory, Upton, NY

Guest Lecturer Nov 2019

- Short Course on X-ray Absorption Fine Structure: Theory, Data Analysis and Modeling
  - Graduate and postgraduate course on the theory and experiment of X-ray absorption spectroscopy and its applications

- Presented sections on *"FEFF9 code for XANES modelling"*, and *"FEFF9 code for XANES modelling (demo)"*

Brookhaven National Laboratory, Upton, NY

Guest Lecturer Nov 2018

- Short Course: Introduction to X-ray Absorption Spectroscopy
  - Graduate and postgraduate course on the theory and experiment of X-ray absorption spectroscopy and its applications
  - Presented sections on *"Theory of XAFS"*, *"FEFF9 code for XANES and EXAFS analyses"*, and *"XANES data analysis with FEFF9 (demo)"*

Univ. de São Paulo, São Carlos, SP, Brazil

Guest Lecturer Mar – Apr 2015

- 1^{st} Brazilian School of X-ray Absorption Spectroscopy
  - Graduate and postgraduate course on the theory and experiment of X-ray absorption spectroscopy and its applications
  - Presented sections on *"Introduction to XANES theory"*, *"XANES with FEFF"*, and *"FEFF demonstration"*

Univ. of Pittsburgh, Pittsburgh, PA

Teaching Assistant Fall 1996

- Instructor in Quantum Mechanics and Kinetics (CHEM 2430)
  - Developed and graded problem sets
  - Taught usage of Computational Chemistry software
  - Managed laboratory for computer experiments

Univ. de la República, Montevideo, Uruguay

Lecturer 1994 – 1996

- Lecturer in Quantum Mechanics and Quantum Chemistry
  - Developed and taught curricula for Basic Quantum Mechanics and Chemistry courses

Instructor 1992 – 1994

- Instructor in Applied Numerical Methods and Programming
  - Taught Pascal programming applied to numerical methods (integration, differential equations, root finding, etc.)

Professional Memberships

- American Physical Society
- International X-ray Absorption Society

Professional Service

Referee Service

- *Physical Review*
- *Journal of the American Chemical Society*
- *Surface Science*
- *Journal of Physical Chemistry*
- *Science*

Service

Finn Hill Middle School Career Day, Apr 2015 and Apr 2019

- Presented: "Becoming a condensed matter theorist (Or "How to play with atoms in a computer")"

Lake Forest Park Elementary School Science Night, Mar 2010
- Managed a booth with hands-on demonstrations of the interaction between light with matter

Hardware and Software Skills

Distributed Cluster Assembly, Maintenance and Administration:
- Collaborated in the construction, configuration and administration of IBM and Linux clusters in the Dept. of Chemistry, Univ. of Pittsburgh
- Requisitioned, administered and maintained the Linux clusters of the Condensed Matter Theory Group in the Dept. of Physics, Univ. of Washington

Computer Programming:
- Fortran, MPI, Python, Pascal, UNIX shell scripting

Numerical Analysis:
- Octave, MATLAB, Mathematica

Version Control:
- Git and CVS

Information/Internet Technology:
- Cloud Computing, Amazon EC2

Desktop Editing and Productivity Software:
- Vim
- LaTeX, BibTeX
- Microsoft Office, OpenOffice.org, Google Docs
- GIMP, InkScape, POVRay

Operating Systems:
- Microsoft Windows family, Linux, BSD, IRIX, AIX, Solaris, and other UNIX variants

Awards

Univ. of Pittsburgh
- Andrew Mellon Predoctoral Fellowship, 1999–2000

References

Reference available upon request.

More Information

More information can be found at
http://staff.washington.edu/fdv