## M. Victoria (Marivi) Fernández-Serra

---


**Personal Data**

DOB: Januray 19th 1976.
Nationality: US.

**Contact Information**

Department of Physics and Astronomy,
Physics and Astronomy department, Stony Brook University.
Institute for Advanced Computational Sciences IACS, Stony Brook University,
Stony Brook, NY 11794-3800, US

*Telephone:* (+1) 631 6328244

*E-mail:* maria.Fernández-Serra@stonybrook.edu

*Web page:* http://mini.physics.sunysb.edu/∼marivi/


**Education**

- **Cambridge University**. U.K.
  - *Ph.D.* , Jesus College, (January, 2002-February, 2005).
    Dissertation Topic: "First-principles characterization of natural matter: Biomolecules and water".
    Advisor: Emilio Artacho (University of Cambridge).
- **Universidad Autónoma de Madrid**, Spain
  - Masters in Condensed Matter Physics (September, 1999 - December 2001).
    Dissertation Topic: "Acceleration of first principles structural relaxations"
    Advisors: Jose M. Soler (Universidad Autónoma de Madrid).
  - BA, Physics, (September, 1994-July, 1999).

**Appointments**

- **Professor** Physics and Astronomy department and Institute for Advanced Computational Sciences, Stony Brook University. Since September 2018
- **Associate Professor** Physics and Astronomy department and Institute for Advanced Computational Sciences, Stony Brook University. September 2013-August 2018
- **Assistant Professor** Physics and Astronomy department and Institute for Advanced Computational Sciences, Stony Brook University. January 2008-August 2013
- **Post-doctoral Associate** Centre Européen de Calcul Atomique et Moléculaire (CECAM), ENS-Lyon. September 2006- December 2007
- **Post-doctoral Associate** Laboratoire de Physique de la Matière Condensée et Nanostructures (LPMCN) et CNRS. Universite Claude Bernard Lyon 1 (France), January 2005-August 2006.

**Honors and Awards**

- 2024: Severo Ochoa Visiting Professor. Catalan Institute for Nanoscience and Nanotechnology May-June 2024.
- 2021: APS Fellow, Division of Computational Physics. For extending density functional theory in groundbreaking work on the structure and dynamics of complex materials, and especially for improving understanding of the electronic structure of water, including ice and interfaces.
- 2010: DOE Early Career Award.
- 2006-2008: Marie Curie Fellowship, with Prof. Berend Smit, CECAM, Lyon France.
- 2002-2004: PhD Fellowship, Cambridge European Trust.

- 2002-2004: PhD Fellowship Environmental and Physical sciences Research Council, UK.
- 2002-2004: PhD Fellowship Comunidad Autonoma de Madrid. Spain.
- 2000-2001: Spanish Research Council (C.S.I.C) Research Fellowship (Master project).
- 1998-1999: Undergraduate Fellowship: Introduction to Research Consejo Superior de Investigaciones Científicas, C.S.I.C. Spain (Spanish Council of Scientific Research).
- 1997-1998: Studentship from the European program Erasmus-Sócrates, Universitá Degli Studi Di Padova.

## Publications

1. " Anti-Coulomb ion-ion interactions: A theoretical and computational study" A Wills, A Mannino, I Losada, SG Mayo, JM Soler, M Fernández-Serra Physical Review Research 6 (3), 033095, 2024
2. "Flexoelectricity and surface ferroelectricity in natural water ice" X. Wen, Q. Ma, A. Mannino, M. Fernandez-Serra, S. Shen1, G. Catalan. Under Review in Nature Physics (2023).
3. "Fully ab-initio all-electron calculation of dark matter–electron scattering in crystals with evaluation of systematic uncertainties", Cyrus E Dreyer, Rouven Essig, Marivi Fernandez-Serra, Aman Singal, Cheng Zhen. arXiv:2306.14944, Phs. Rev. D 2023.
4. "Dark matter direct detection with quantum dots" Carlos Blanco, Rouven Essig, Marivi Fernandez-Serra, Harikrishnan Ramani, Oren Slone, Physical Review D 107 (9), 095035., 2023
5. "Quantum Phase Transition Predicted for Gaseous Water" M Fernandez-Serra Physics 16, 5, 2023.
6. "Skipper-CCD sensors for the Oscura experiment: requirements and preliminary tests" BA Cervantes-Vergara, S Perez, J Estrada, A Botti, CR Chavez, ...,Fernandez-Serra... (Oscura Collaboration). Journal of Instrumentation 18 (08), P08016. 2023
7. "Cooperative Interactions between Surface Terminations Explain Photocatalytic Water Splitting Activity on $SrTiO_3$" Vidushi Sharma, Benjamin Bein, Amanda Lai, Betül Pamuk, Cyrus E. Dreyer, Marivi Fernández-Serra, and Matthew Dawber, PRX Energy 1, 023002.
8. "Using Neural Network Force Fields to Ascertain the Quality of Ab Initio Simulations of Liquid Water", Alberto Torres, Luana S. Pedroza, Marivi Fernandez-Serra and Alexandre R. Rocha, The journal of Physical Chemistry B, https://doi.org/10.1021/acs.jpcb.1c04372 2021.
9. "Highly accurate and constrained density functional obtained with differentiable programming", Sebastian Dick and Marivi Fernandez Serra, Phys. Rev. B 104, L161109 (2021)
10. "Role of Water Model on Ion Dissociation at Ambient Conditions", Alec Wills and Marivi Fernandez Serra, The Journal of Chemical Physics 154, 194502 (2021). DOI:10.1063/5.0046188.
11. "Proton-transfer dynamics in ionized water chains using real-time Time Dependent Density Functional Theory," Vidushi Sharma, Marivi Fernández-Serra. Phys. Rev. Research 2, 043082, 2020
12. "Machine Learning a Highly Accurate Exchange and Correlation Functional of the Electronic Density", Sebastian Dick and Marivi Fernandez-Serra, Nat Commun 11, 3509 (2020).
13. "LBECA: A Low Background Electron Counting Apparatus for Sub-GeV Dark Matter Detection", A. Bernstein, M. Clark, R. Essig, M. Fernandez-Serra, A. Kopec, R.F. Lang, J. Long5, K. Ni, S. Pereverzev, J. Qi, P. Sorensen, J. Xu, J. Ye and C. Zheng. 2020 J. Phys.: Conf. Ser. 1468 012035

14. "Water-induced formation of an alkali-ion dimer in cryptomelane nanorods". Shaobo Cheng, Vidushi Sharma, Altug S. Poyraz, Lijun Wu, Xing Li, Amy C. Marschilok, Esther S. Takeuchi, Kenneth J. Takeuchi, Marivi Fernandez-Serra and Yimei Zhu. Chemical Science, 2020, DOI: 10.1039/D0SC01517B
15. "Learning from the density to correct total energy and forces in first principle simulations" Sebastian Dick and Marivi Fernandez-Serra, J. Chem. Phys. 151, 144102 (2019).
16. "Using a monomer potential energy surface to perform approximate path integral molecular dynamics simulation of ab initio water at near-zero added cost" DC Elton, M Fritz, M Fernandez-Serra, Phys. Chem. Chem. Phys., 2019,21, 409-417.
17. "Atomic Scale Account of the Surface Effect on Ionic Transport in Silver Hollandite" X Hu, J Huang, L Wu, M Kaltak, MV Fernandez-Serra, Q Meng, L Wang, Amy C Marschilok, Esther S Takeuchi, Kenneth J Takeuchi, Mark S Hybertsen, Yimei Zhu. Chemistry of Materials 30 (17), 6124-6133
18. "Unveiling two types of local order in liquid water using machine learning", Adrian Soto, Deyu Lu, Shinjae Yoo,and Marivi Fernández-Serra, arXiv:1707.04593 submitted to *J. Chem. Phys.* (2019)
19. "Insights into the Structure of Liquid Water from Nuclear Quantum Effects on the Density and Compressibility of Ice Polymorphs" B Pamuk, PB Allen, MV Fernández-Serra. The Journal of Physical Chemistry B 122 (21), 5694-5706, (2018)
20. "Charge localization and ordering in hollandite group oxides: Impact of density functional theory approaches" M Kaltak, M Fernández-Serra, MS Hybertsen Physical Review Materials 1 (7), 075401, 2017
21. "How water's properties are encoded in its molecular structure and energies" Emiliano Brini, Miha Lukvsivc, Christopher J. Fennell, Barbara Hribar-Lee, Marivi Fernández-Serra and Ken Dill, *Chemical Reviews*, in press (2017) DOI: 10.1021/acs.chemrev.7b00259
22. "Bias-dependent local structure of water molecules at a metallic interface", Luana S. Pedroza, Pedro Brandimarte, Alexandre Reily Rocha, Marivi Fernández-Serra, *Chemical Science*, Chemical Science, 2018, DOI: 10.1039/C7SC02208E.
23. "Visualization of lithium-ion transport and phase evolution within and between manganese oxide nanorods" Feng Xu, Lijun Wu, Qingping Meng, Merzuk Kaltak, Jianping Huang, Jessica L. Durham, Marivi Fernández-Serra, Litao Sun, Amy C. Marschilok, Esther S. Takeuchi, Kenneth J. Takeuchi, Mark S. Hybertsen and Yimei Zhu. Nature Communications 8, Article number: 15400 (2017) doi:10.1038/ncomms15400
24. "Coupling of bias-induced crystallographic shear planes with charged domain walls in ferroelectric oxide thin films", LMyung-Geun Han, Joseph A. Garlow, Matthieu Bugnet, Simon Divilov, Matthew S. J. Marshall, Lijun Wu, Matthew Dawber, Marivi Fernández-Serra, Gianluigi A. Botton, Sang-Wook Cheong, Frederick J. Walker, Charles H. Ahn, and Yimei Zhu. doi/10.1103/PhysRevB.94.100101 Phy. Rev. B (Rapid Comm.), 2016
25. "First-principles study of pyroelectricity in GaN and ZnO", Jian Liu, Maria V. Fernández-Serra, and Philip B. Allen, *Phys. Rev. B* **93**, 081205(R) (2016)
26. "Continuous melting through a hexatic phase in confined bilayer water", Jon Zubeltzu, Fabirano Corsetti, M.-V. Fernández-Serra, Emilio Artacho, *Phys. Rev. E* (2016), DOI: 10.1103/PhysRevE.93.062137
27. "Optimization of an exchange-correlation density functional for water", Michelle Fritz, Marivi Fernández-Serra and Jose M. Soler, *J. Chem. Phys.* **144**, 224101 (2016)
28. "First-principles study of pyroelectricity in GaN and ZnO", Jian Liu, Maria V. Fernández-Serra, and Philip B. Allen, *Phys. Rev. B* **93**, 081205(R) (2016)
29. "Special quasiordered structures: Role of short-range order in the semiconductor alloy (GaN) 1 x (ZnO) x" J Liu, MV Fernández-Serra, PB Allen Physical Review B 93 (5), 054207

30. "The hydrogen-bond network of water supports propagating optical phonon-like modes", D. Elton and M. V. Fernández-Serra, Nature Communications 7, Article number: 10193, (2016)
31. "Direct Detection of sub-GeV Dark Matter with Semiconductor Targets", R. Essig, J. Mardon, M. V. Fernández-Serra, A. Soto, T. Volansky and T-T. Yu, *Journal of High Energy Physics*, 2016(5), 1-54
32. "GW and Bethe-Salpeter study of small water clusters", X. Blase, Paul Boulanger, Fabien Bruneval, Marivi Fernández-Serra, and Ivan Duchemin. *J. Chem. Phys.* **144**, 034109 (2016)
33. "Electronic and nuclear quantum effects on the ice XI/ice Ih phase transition" B. Pamuk, P. B. Allen and M. V. Fernández-Serra, *Phys. Rev. B* **92**, 124105 (2015)
34. "Local order of liquid water at metallic electrode surfaces" Luana Pedroza, A. Poisier and M. V. Fernández-Serra, *J. Chem. Phys*, **142** , 034706 (2015)
35. "Optimal finite-range atomic basis sets for liquid water and ice" Fabiano Corsetti, M.-V. Fernández-Serra, José M. Soler, and Emilio Artacho, J. Phys.: Condens. Matter 25 (2013) 435504.
36. "Room temperature compressibility and the diffusivity anomaly of liquid water from first principles". Fabiano Corsetti, Emilio Artacho, José M. Soler, S. S. Alexandre, M.-V. Fernández-Serra, J. Chem. Phys. 139, 194502 (2013).
37. "Polar nanoregions in water - a study of the dielectric properties of TIP4P/2005, TIP4P2005f and TTM3F", Daniel C. Elton, M. V. Fernández-Serra, *J. Chem. Phys*, **140** , 124504 (2014).
38. "Temperature and composition dependence of short-range order and entropy, and statistics of bond length: the semiconductor alloy (GaN)1-x(ZnO)x", Jian Liu, Luana S. Pedroza, Carissa Misch, Maria V. Fernández-Serra, Philip B. Allen, *J. Phys. Cond. Matter*, **26**, 274204 (2014).
39. "Are the anomalies in water due to an unapproachable critical point? " Commentary by M.V. Fernández-Serra for the Journal Club for Condensed Matter Physics., April 2013.
40. "Quantum zero point effects using modified Nose-Hoover thermostats." Sriram Ganeshan, R. Ramirez, and M. V. Fernández-Serra, *Phys. Rev. B.* **87**, 134207 (2013).
41. "Effects of electronic correlation, physical structure, and surface termination on the electronic structure of $V_2O_3$ nanowires". Amanda L. Tiano, Jingbin Li, Eli Sutter, S. Wong and M.V. Fernández-Serra. *Phys. Rev. B.* **86**, 125135 (2012).
42. "Quasi-harmonic approximation of thermodynamic properties of ice Ih,II, and III" R. Ramirez, N. Neuerburg, M. V. Fernández-Serra, and C. Herrero. *J. Chem. Phys.* **137**, 044502 (2012).
43. "Water dissociation at the GaN(10-10) surface: structure, dynamics and surface acidity" Jue Wang, Luana Pedroza, Adrien Poissier and M. V. Fernández-Serra, *J. Phys. Chem. C*,**116** (27), pp 14382-14389, (2012).
44. "Ferroelectric $PbTiO_3/SrRuO_3$ superlattices with broken inversion symmetry." S.J. Callori, J. Gabel, D. Su, J. Sinsheimer, M.-V. Fernández-Serra and M. Dawber. *Phys. Rev. Lett.* **109**, 067601 (2012).
45. "Anomalous nuclear Quantum Effects in Ice" B. Pamuk, J. M. Soler, R. Ramirez, C. P. Herrero, P. W. Stephens, P. B. Allen, and M.-V. Fernández-Serra. *Phys. Rev. Lett.* **108**, 193003 (2012).
46. " Ab initio study of charge doping effect on 1D polymerization of $C_{60}$". R. Poloni, A. San Miguel and M.V. Fernández-Serra. *J. Phys. Cond. Matt.* , **24**, 095501 (2012).
47. "Electronic Transport in Natively Oxidized Silicon Nanowires" Mohammad Koleini, Lucio Colombi Ciacchi, and M.-V.Fernández-Serra. *ACS Nano*, **5 (4)**, 28392846, (2011).
48. "Density, structure and dynamics of water: the effect of Van der Waals interactions", Jue Wang, G. Roman-Perez, Jose M. Soler, Emilio Artacho, and M.-V.Fernández-Serra, *J. Chem. Phys.* **134**, 024516 (2011).
49. "The role of hydrogen bonding in water-metal interactions" Adrien Poissier, Sriram Ganeshan, and M. V. Fernández-Serra. *Phys. Chem. Chem. Phys.* 3375-3384 (2011).

50. "Substrate-induced cooperative effects in water adsorption from density functional calculations" Pepa Cabrera-Sanfelix, M. V. Fernández-Serra, A. Arnau, and D. Sanchez-Portal. *Phys. Rev. B*,**82**, 125432 (2010).
51. "Photocatalytic Water Oxidation Process at the GaN (1010) - Water Interface" Xiao Shen, Yolanda A. Small, Jue Wang, Philip B. Allen, M. V. Fernández-Serra, Mark S. Hybertsen, and James T. Muckerman, 2010, *J. Phys. Chem. C*, **114**, 13695 (2010).
52. "Conductance of functionalized nanotubes, graphene and nanowires: from ab initio to mesoscopic physics". Blase, C. Adessi, B.Biel, A. Lopez-Bezanilla, M.V. Fernández-Serra, E.R. Margine, F. Triozon and S.Roche. *Physica status solidi* ,(b), n/a. doi: 10.1002/pssb.201000135.
53. "Radial breathing mode in silicon nanowires: An ab initio study" E. Bourgeois, M.-V. Fernández-Serra, and X. Blase, *Phys. Rev. B*, **81**, 193410 (2010).
54. "Melting the world's smallest raindrop" M. V. Fernández-Serra. *Physics*, **2**, 67 (2009).
55. "Zone-center instability of C(5,0) carbon nanotubes inside $AlPO_4$-5 channels" M.V. Fernández-Serra, X. Blase. *Phys. Rev. B*, **77**, 195115 (2008).
56. "High-pressure stability of Cs6C60 " R. Poloni and D. Machon and M. V. Fernández-Serra and S. Le Floch and S. Pascarelli and G. Montagnac and H. Cardon and A. San-Miguel. *Phys. Rev. B*, **77**, 125413 (2008).
57. "Preserved Conductance in Covalently Functionalized Silicon Nanowires" X. Blase and M. V. Fernández-Serra. *Phys. Rev. Lett.*, **100**, 046802 (2008).
58. "Pressure-induced deformation of the C60 fullerene in Rb6C60 and Cs6C60" R. Poloni, M. V. Fernández-Serra, S. Le Floch, S. De Panfilis, P. Toulemonde, D. Machon, W. Crichton, S. Pascarelli, and A. San-Miguel. *Phys. Rev. B*, **77**, 035429 (2008).
59. "Conductance, surface traps and passivation in doped silicon nanowires" M.V. Fernández-Serra, Ch. Adessi, X. Blase. *Nanoletters* , **6**, 2674 (2006).
60. "Surface segregation and backscattering in doped silicon nanowires" M.V. Fernández-Serra, Ch. Adessi, X. Blase. *Phys. Rev. lett.*, **96**, 166805 (2006).
61. "Electrons and hydrogen-bond connectivity in liquid water", M.V Fernández-Serra and E. Artacho. *Phys. Rev. Lett*, **96**, 016404 (2006).
62. "Electronic structure of semiconducting nanowires" Y.M. Niquet, A. Lherbier, N.H. Quang, M.V. Fernández-Serra, X. Blase, Ch. Delerue. *Phys. Rev. B*, **73**, 165319 (2006).
63. "Novel structural features of CDK inhibition revealed by an ab initio computational method combined with dynamic simulations" L. Heady, M.V Fernández-Serra ,R. L. Mancera, S. Joyce, A. R. Venkitaraman, E. Artacho, C. K Skylaris, L. C. Ciacchi, and M. C. Payne. *J. Med. Chem*, **49**, 5141 (2006).
64. "Two exchange-correlation functionals compared for first-principles liquid water", M.V Fernández-Serra, G. Ferlat and E. Artacho. *Mol. Sim.*, **31**, 361-366 (2005).
65. "Network equilibration and first principles liquid water", M.V Fernández-Serra and E. Artacho. *J. Chem. Phys.* **121**, 11136-11144 (2004).
66. "Model Hessian for accelerating ab-initio geometry optimizations", M.V Fernández-Serra, E. Artacho and J. M. Soler. *Phys. Rev. B. Rapid Comm.*, **67**, 100101 (2003).
67. "Electron density in the peptide bonds of crambin", M. V. Fernández-Serra, J. Junquera,C. Jelsch, C. Lecomte and Emilio Artacho, *Solid St. Commun.*, **116**, 395-400 (2000).

*Book Chapters*

– "Electronic and Transport Properties of Silicon Nanowires". M.v Fernández-Serra and X. Blase. The Oxford Handbook on Nanoscience and Technology Vol 1: Basic Aspects. Oxford University press, 2010. ISBN 978-0-19-953304-6.

Invited Oral Presentations.

- Artificial Intelligence for Advanced Materials, AI4AM2025, San Sebastian (Spain): April 08-10, 2025
- APS March Meeting Mar 16–21, 2025 Anaheim, CA
- Plenary Speaker: VII Colloquium on Computational Simulation in Sciences, August 26 - 30, 2024, UNAM
- 2024 Lawrence Livermore National Laboratory Computational Chemistry and Materials Science Summer Institute (CCMS), July 2024/
- Workshop on Machine Learning in Electronic-Structure Theory, March 25 to 29, 2024 at the Institute for Mathematical and Statistical Innovation, University of Chicago.
- IPAM Reunion Workshop December 2023.
- PHYMOL2023, Luxemburg, September 2023.
- 62nd Sanibel Symposium, February 2023
- APS March Meeting March 2023.
- Korean Physical Society 2022, Pioneer Symposium, Machine Learning for First-Principles Calculations. Oct 20-21 2022
- ACTC 2022, Lake Tahoe, July 25-28 2022
- Telluride Workshop: Multi-Scale Quantum Mechanical Analysis of Condensed Phase Systems: Methods and Applications, July 12-13 2022.
- Electronic Structure 2022, NYC June1-4.
- IPAM Workshop, Monte Carlo and Machine Learning Approaches in Quantum Mechanics" May 23-27.
- IPAM Fellow, program Mathematics and quantum Mechanics 2022.
- Telluride Workshop Water Grand Challenges, NY 2021
- APS March meeting 2021
- Machine Learning in Quantum Physics, NY 2021
- Pacifichem 2020, Honolulu, Hawaii December 2020.
- American Conference on Theoretical Chemistry (ACTC),Lake Tahoe (virtual) July 26 - 30, 2020
- Machine Learning for quantum Simulatins Virtual Conference, June 2020, CCQ, NY.
- "Machine learning density functionals" ISTCP-X 2019, July 2019, Norway.
- "Ab initio modeling of anion-cataion association in water: unravelling the effects of sampling, water structure and charge localization in the the structure and dynamics of the ion pairs" Telluride water conference, June 2019
- "More Efficient and Accurate DFT-based Dynamics via Machine Learning", MMM Hub Conference London, September 2018
- "Evaluating photocatalytic active sites as function of polarization, level alignment and spontaneous dissociation of hydroxyl groups at perovskite oxide surfaces", invited talk at ACS 256th National Meeting in Boston, August 2018.
- "Understanding liquid water from first principles: a tale of two liquids", invited talk at the American Physical Society MAS Meeting, Nov 3 - 5 2017.

- "Dark matter detection problem and how electronic structure methods can help", invited talk at IACS - TIT (Tokyo Institute of Technology) scientific meeting, Oct 15 2017.
- "Interplay between surface termination and polarization in photocatalysis on perovskite oxide surfaces", invited talk at ACS 254th National Meeting in Washington DC, August 2017.
- "Development of new density functionals and new methods for analysis of convergence of ab initio molecular dynamics simulations", invited talk at the Recent Developments in Electronic Structure Theory, Princeton June 2017.
- "Computational modeling in condensed matter physics: from water to Dark matter", invited talk at the APS march meeting, New Orleans March 2017.
- "Development of new density functionals and new methods for analysis of convergence of ab initio molecular dynamics simulations". ACS 2016 Northeast Regional Meeting (NERM), Binghamton, NY, October 5-8, 2016
- "Development of new density functionals and new methods for analysis of convergence of ab initio molecular dynamics simulations". ACS 2016 Advanced Potential Energy Surfaces Symposium (PHYS division) in Philadelphia, August 21-25, 2016.
- "Link between photocatalytic water splitting efficiency and surface acidity in GaN and SrTiO3". APS March Meeting, San Antonio TX, March 2015.
- Nordita Water School October 2014: Coordinator of Ab Initio Simulations Group.
- Invited oral presentation at Water2014, Metastabilty and Nucleation in water, Les Houches June-16 2014.
- Invited presentation at: WATER-Europe Conference. Zaragoza, Spain, June 2014.
- Local order of liquid water at the electrochemical interface, Invited presentation, 2014 Sanibel Symposium, Fl, February 17 2014.
- "Water structure and redox level alignment at the water/semiconductor interface from first principles". Invited Oral presentation at the 246th ACS National Meeting, Indianapolis, Indiana, September 8-12, 2013.
- M.V Fernández-Serra:" Water structure and redox level alignment at the water/semiconductor interface from first principles " Invited Oral presentation to be presented on 28 August 2013. SPIE Solar Energy + Technology 25 - 29 August 2013 in San Diego, California.
- "LDL/HDL fluctuations in liquid water". 7th international discussion meeting on ralaxations in Complex Systems: Water and Hydrogen bonded Systems. July 21-16 2013.
- "Charges on the edge: Quantum signatures in the structure of water". 2012 Water and Aqueous Solutions Gordon Research Conference. August 12-17 2012.
- "van der Waals interactions in water and ice from density functional theory simulations: improvements and challenges". APS March meeting 2012, March 18-13 2012, Boston.
- "Water dissociation and dynamics on photocatalytic surfaces: link between surface chemistry of water and photocatalysis." 243rd ACS National Meeting, March 25 - March 29, 2012, San Diego.
- "Anomalous nuclear Quantum Effects in Ice." Workshop MINI 2012, Computational materials science and nanoscience from first principles. Barcelona, January 12-14, 2012.
- "Electric boundary conditions in first principles molecular dynamics simulations: Water polarization under short circuit electrodes" Cecam Workshop on Molecular Simulation in External Electric and Electromagnetic Fields. May 19, 2011 to May 21, 2011. University College Dublin, Ireland .
- "Water dissociation and dynamics on GaN surfaces: link between surface chemistry of water and photocatalysis." Materials Research Society fall meeting at Boston, December 2010.

- "Water structure and dynamics at catalytic semiconductor and metallic interfaces from first principles." "French-American Young Engineering Scientist Symposium" SOLEIL synchrotron Facility in Paris from Nov. 16-18, 2009.
- "Water structure and dynamics at catalytic semiconductor and metallic interfaces from first principles." 6th annual meeting on Condensed Phase and Interfacial Molecular Science (CPIMS), Oct 19-21, 2009 Virginia.
- " Water structure and dynamics at catalytic semiconductor and metallic interfaces from first principles." "The Physical Chemistry of Photon to Fuel Conversion", National ACS Meeting on August 16-22, 2009 in Washington, DC.
- " Electronic structure and dynamics of liquid water within local orbital representation" "Advances in Electronic Structure Theory and First Principles Dynamics", National ACS Meeting March 22-26, 2009 in Salt Lake City, Utah.
- "Electronic transport in doped and functionalized silicon nanowires". CECAM Workshop on "Structural, electronic and transport properties of quantum wires", CECAM, Lyon, 9-12 June 2008.
- "Conductance, surface traps and passivation in doped silicon nanowires". NanoSpain Workshop , Sevilla 12-15 march, 2007.
- "Conductance, surface traps and passivation in doped silicon nanowires". CECAM Workshop on "Quantum Transport and non-adiabatic electron evolution from first principles approaches", CECAM, Lyon, 4-8 Dec. 2006.
- "First principles characterization of liquid water" *Psi-k* 2005 Conference, Schwabisch Gmund, Germany, September 17 - 21, 2005
- "Model Hessian for accelerating ab-initio geometry optimizations", Tenth International Conference in Total Energy Methods, Tenerife 10-12 January 2002, Spain.

## Invited Seminars and Colloquiums

- ICN2 Thursday, 30 May 2024. Designing exchange and correlation functionals for DFT using Machine learning: Theory and Practical Implementation
- University of Michigan Ann Harbor Physics Colloquium January 2024
- Duke Materials Science Colloquium May 2023
- New York University, Physics Graduate Colloquium Feb 2022
- University of Texas El Paso, Colloquium Feb 2022
- Princeton University CSI Seminars Dec 2021
- Temple University, Physics Colloquium, October 2019
- Princeton University Chemistry department seminar, February 2019
- Central Michigan University, Physics Colloquium, October 2018
- University of Minnesota, Materials Sciences Colloquium, October 2018
- Rutgers University, Condensed Matter Physics Colloquium, October 2017.
- Harvard University, Applied Physics Colloquium, February 2017.
- Universidad Autonoma de Madrid, Physics Colloquium, May 2016.
- Donostia International Physics Center, San Sebastian, Spain. January 2015.
- Invited colloquium ICMAB, Barcelona, Spain. May 2015
- Nordita Water School October 2014: Coordinator of Ab Initio Simulations Group.
- Stony Brook Worlds of Physics, November 2013.
- Oak Ridge National Laboratory, Neutron Spallation Source Colloquium, September 2013.
- Harvard University. ITAMP joing quantum Seminar, December 7, 2012.

- University of South Dakota. Chemistry Colloquium, January 2013.
- University of Madison. Theoretical chemistry colloquium, November 2011.
- The Worlds of Physics, Stony Brook University, March 2010.
- The Worlds of Physics, Stony Brook University, September 2009.
- Colloquium, Physics Department, Wesleyan University, October 2009.
- Colloquium, Physics Department, The College of New Jersey, September 2009.
- Invited Physics Seminar, ICMAB, CSIC, Barcelona, June 2009.
- Invited Physics Seminar, Brookhaven National Laboratory, September 2008.
- Colloquium, Chemistry department Stony Brook University, May 2008.
- Colloquium, "Structure and dynamics of the hydrogen bond network: from bulk water to ice and water at interfaces". DIPC, San Sebastian, Spain. November 2007.
- Invited Physics Seminar, Stony Brook University, January 2007.
- Invited Physics Seminar, Brookhaven National Laboratory, January 2007.

## International Committees and Panels and Conference Organization

- Elected Secretary-Treasurer DCOMP (2023-2026)
- Molecular Foundry Theory Facility Reviewer. 2022-present,.
- Advisory Board Member AMEWS EFRC (Argonne) 2021-present
- Advisory Board Member Flosic center at Central Michigan University (2021-present).
- Judge, 2023-2024 Blavatnik Regional Awards for Young Scientists.
- Elected Secretary-Treasurer DCOMP (2021-2023)
- (IPAM) Spring 2022 Program on Advancing Quantum Mechanics with Mathematics and Statistics.
- Chair: Telluride Water Grand Challenges is Science and Engineering 2021 Conference.
- APS March meeting Focus session organizer: Modeling the electrochemical interface and aqueous solutions. 2018-2024
- Chair Metropolis award prize 2020
- Chair APS DCMP Fellowship Committee 2022
- Chair Telluride water conference 2021
- Elected Member at Large DCOMP (2017-2019)
- Elected Member at Large DCMP (2019-2021)
- Advisory Visiting Committee for Physical Review Letters editorial Board. September 2013.
- Linac Coherent Light Source (LCLS), SLAC, Stanford, Proposal Review Committee. Member 2012-2015.
- Division of Computational Condensed Matter Physics, DCOMP, APS. Elected member at large, May 2016-May 2019
- DCOMP, APS, nomination committee member May 2017-2019
- Correspondent member Condensed Matter Physics Journal Club, 2015-2020.
- DOE Exascale Requirements Review, November 2015.
- ASCR Leadership Computing Challenge (ALCC) Panel Review. April 2016.
- ASCR Exascale Requirements Crosscut Review Tyson, VA, March 9-10, 2017.
- Basic Energy Sciences (BES) Roundtable on Opportunities for Quantum Computing in Chemical and Materials Sciences. October 2017

- BES Early Career Review panel 2011-2019.

## Teaching Experience

- Graduate Level: PHY 546, Python for scientific programming. (Spring 2019)
- Graduate Level: PHY 555, Solid State Physics (Fall 2008,2009,2010,2012, 2018-2021)
- Undergraduate Level: PHY277, Computation for Physics and Astronomy (Spring 2009,2010,2011,2012,2013,2017)
- Undergraduate Level: PHY306, Thermal Physics (Spring 2013,2014, 2015,2018)
- Undergraduate Level: PHY313, The Physics of Water (Fall 2011)
- Undergraduate Level: PHY141, PHY142 (22021-present),PHY132 (Spring and Fall 2016)

## Outreach Activities

- Organizer IACS Challenge. A competition for K12 students showcasing the role of women in science. 2023-2024
- Coordinator, The Worlds of Physics, Stony Brook University: Monthly Physics Seminars for the general audience. (2010-2017)
- High School Students Mentoring, Simon's Fellows mentoring:
  - 2008: Jordan Tung (Simon Fellow). Now at MIT.
  - 2009: Erica Lai (Simon Fellow). Siemens and Intel Competitions Semifinalist. Now at MIT
  - 2010: Michael Ladevaia.
  - 2013: Jessie Hsiao. Now at MIT.
  - 2017: Nathan Geist.

## Professional Activities

- Membership: American Physical Society (APS), American Chemical Society (ACS)
- Editorial Review: Phys. Rev. Lett, Phys. Rev. B, EuroPhys. Lett., J. Am. Chem. Soc, J. Phys. Chem. (A and B)., Nanoletters, App. Phys. Letters, Nature, Nature Comm., Chem. Sci
- Proposal Review: NSF (condensed Matter and Materials Physics), DOE, NSF CDI panel.
- Physics Department Service: Status of Women committee (2010-2018), Quality of Life Committee (2010-present), Condensed Matter Theory search (2010,2011, 2017). Mentoring committee (2018-present). Coloqium Committee Chair (2019-present). Strategic and Long Range Planing Committee Chair (2020). Strategic Hiring initiatives Chair (2022-present).
- IACS Service: Diversity committee (standing), Recruitment (standing), IACS Fellowship(standing). IACS Endowed Hires committee (2019-2020).
- University Service: University Senior PTC committee (2022-present). Member, Middle States Accreditation Reaffirmation Committee (2023-2024).

## Graduate Students

- Meg Hott(2024-present)
- Aman Singal (2021-present)
- Anthony Manino (2021-present)
- Kedarsh Kaushik (2021-present)
- Aman Singal (2021-present)
- Alec Wills (2018-2024)
- Sebastian Dick (2017-2021)
- Vidushi Sharma (2016-2021

- Simon Divilov (2013-2018)
- Adrian Soto-Cambres (Graduated Aug 2017)
- Daniel Elton (2012-2016)
- Dhruv Mittal (Masters, graduated Jun 2016)
- Jonathan Siebert (Masters, graduated Aug 2014)
- Betul Pamuk (Graduated Summer 2014)
- Sriram Ganeshan (Graduated summer 2012)
- Jue Wang (Graduated summer 2011)
- Adrien Poissier (Graduated, December 2011)
- Judith Gabel (Masters, graduated Aug 2011)

Post-doctoral Associates

- Dr Merzuk Kaltak (2016-2017)
- Dr Luana Pedroza (2011-May 2014).