Mark R Pederson, Ph.D.

Employment History, Sabbaticals, and Government Service

2019-Present	**Professor and Chair**, Department of Physics, The University of Texas at El Paso.
2008-2019	**Program Manager (2008-2016) then Founding Program Manager (2017-2019)** of the DOE Office of Science Computational and Theoretical Chemistry Program (Washington DC).
2013-2017	**Research Professor**, Department of Chemistry, John Hopkins University (unpaid).
2002-2003, 2007-2008	**Program Officer**, National Science Foundation, Theoretical and Computational Chemistry (2002-2003) and Materials Theory (2007-2008), NRL Assignment.
Summer 1997	**Visiting Professor**, Department of Physics, Chemnitz Technical Institute (Germany), NRL Assignment.
1992-1993	**Sabbatical**, Max-Planck Institute for Solid State Research, (Stuttgart Germany) (NRL Assignment).
1988-2008	**Research Physicist and Supervisory Research Physicist** Center for Computational Materials Sciences Naval Research Laboratory (Washington DC).
1986-1988	**Postdoctoral Researcher** Naval Research Laboratory (Washington DC), Advisor: Barry M. Klein.

Education

1981-1986	**Ph.D. Atomic, Molecular and Solid State Physics , University of Wisconsin Madison** Thesis title: *Orbital Dependent Improvements of the Density Functional Formalism, Advisor: Prof. Chun C. Lin*
1977-1981	**B.S. Physics, University of Michigan - Ann Arbor** UG Research Areas: *Microwave Resonators (Parity Violation Experiments, Advisors: Bill Williams and Carl Wieman, Random Number Generators for Rare Events (Michigan Proton Decay Experiment, Advisors: Richard Bionta and Larry Sulak.*

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University Services at UTEP

1. Successfully developed a Physics PhD Program with an emphasis on Quantum Science. Starts in August 2024 with a cohort of fourteen new students.
2. Worked on Institutional Transformation Project with Dr. Ann Gates and Veronica Carillo.
3. Member of Sea Change Committee.
4. Serving on university committee to analyze and improve faculty evaluation rubrics led by Dr. Ann Gates and Veronic Carillo.
5. Oversee use of several student support endowments for physics department.

6. Participate in CoS Advisory Board meetings twice per year.
7. Have led the physics' department interactions for many visits by Agencies. An incomplete list is:
   (a) Quantum Science and Computing Presentation, Visit by US Army to UTEP (Fall 2019).
   (b) One-Day PNNL-UTEP Symposium, Visit by PNNL to UTEP, February 19, 2020.
   (c) Many strategy sessions with Mr. Eduardo Monarez (PNNL), 2019-2024.
   (d) Two visits by Dr. Joseph (Airforce) to PNNL, 2020 and 2023.
   (e) Key Note Welcome and Organizer for Office-of-Science Visit to UTEP (February 2024).
   (f) Visit by Space Force
   (g) Prepared justification for a Clare-Luce Boothe Professor of Physics in collaboration with Tami Keating and Dr. Gates (July 2022). MRP is very proud to have developed and maintained an excellent track record for supporting inclusive excellence and workforce recruitment from all segments of society (1988-Present).

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National Panels, Study Sections, and Organizational Activities

1. Spring 2020 NSF Committee of Visitors for Chemistry Division.
2. Office of Advanced Scientific Grand Challenge Computing Allocation Panel (Fall 2020, 2021, 2022, 2023).
3. **2020-2021**: Co-organizer (w/ Jan Musfeldt and Tirol Burrel) of APS March Meeting DMP Focus Session on Multiferroics. (Approximately 5 invited talks and 50 contributed talks).
4. Crosscutting Theory Lead, The Molecular Magnetism and Quantum Materials Energy Frontier Research Center (Fall 2021-Present).
5. **May 2022:** Strong Participation in organizing and moderating the Hispanic Serving Institution Summit for the *NSF Strategic Innovation Summit Series for Advanced Research and Instruction in Artificial Intelligence and Quantum Information Sciences* (Lead by Damon Tull with active input from Dr. Ann Gates). Suggested and introduced key-note speaker and moderated session entitled "Establishing QIS Programs - Overcoming Administrative Barriers".
6. **2021-2022**: Co-Organizer American Chemical Society Spring 2022 Symposium entitled "**New Quantum Solutions for Quantum Systems and Devices**" (Co-Organizer: Professor Laura Gagliardi) See: `https://acs.digitellinc.com/p/s/new-quantum-solutions-for-quantum-systems-and-devices-quantum-algorithms-463161` (Approximately 40 invited talks).
7. **2022-2023:** Coorganizer for the GMAG Symposium of Low Dimensional Magnetism for the 2024 APS March Meeting (Approximately 30 contributed and 5 invited talks).

Classes Taught

I have taught and arranged for graduate seminar 5195 (9 times) and 6195 (2 times). This entails bringing emminent researchers to UTEP for seminars. I have taught Physics Writing (5393) (1), DFT A-Z (5393) (w/T Baruah and R Zope) (1), Mathematical Physics, 4353 (2), Quantum Programming (5393) (1), Spin Physics (5393) w/T Baruah, Vibrational and Core-Level Spectroscopy (5393) with T Baruah and E Kim. Many of the Special Topics classes were taught as precursors to classes at the PhD Level.

Recruitment and Supervision of Scholars:

- **Hired the following professors:** Dr. Yun Pil Shim (2020), Dr. Eunja Kim (2022), Dr. Kedron Silsbee (2023), Dr. Md Fhokrul Islam (2024). PI on Regents Excellence Proposal that will lead to the hire of two new professors in Quantum Information Sciences and two new professors in Clean-Energy Physics. Two of these will be tenured or tenure-track positions and two will be three-year research professorships.
- Developed partnership in Quantum Computing with Linneaus University in Sweden.
- Recruited two sabbatical visitors (Dr. Daniel Finkenstadt, US Naval Academy) and Dr. Winfred Muelwa (University of Egerton, Kenya) for 2024-2025. These faculty are each providing 60-75 percent of their support.
- **Primary Advisor to the following MS graduates students:** Karma Dema (MS 2022), Alex Johnson (MS 2022), Gustavo Bravo Flores (MS 2023), Peter Lasode (MS 2023), Dimuthu Muthunayakage (current). Have committed to advise 2-3 incoming graduate students.
- **Supervised the following postdoctoral students:** Dr. Zahra Hooshmand (2020-2023, now at Microsoft), Dr. Chandra Shahi (2019-2020, now at Tulane University), Dr. Md Fohkrul Islam (2022-2023, Now at Central Michigan University), Dr. Kushantha Withanage (current), Dr. Jesus Nain Pedroza (current).

Funding:

Since coming to UTEP in 2019, Dr. Pederson been awarded approximately $5.6M ofsupport that is primarily used for salary support for students, postdocs, and summer faculty.

Funding Instrument	Agency	PI	Co-PI	Total	Physics Share	MRP's Share
Faculty Startup	Texas STARS and UTEP	Pederson		$1000K	$1000K	$1000K
LDRD[1]	DOE PNNL	Pederson	—	$90K	$90K	$90K
LDRD[2]	DOE PNNL	Pederson	Baruah	$94K	$94K	$47K
MMQM	DOE UFL	Pederson	—	$610K	$610K	$610K
FLOSIC[a]	DOE CMU	Baruah	Pederson	$1948K	$1948K	$828K
NSEC	DOE NNSA	Kim	Pederson	$860K	$860K	$210K
Transd	AFORS	Roberts	Pederson	$1200K	$600K	$150K
ISSR	UTEP	Baruah	Pederson	$149K	$74K	$40K
Tec[4]	DOE PNNL	Pederson	Baruah	$400K	$400K	$200K
NSF	MRI Grant	Gates	Pederson	$700K	$20K	
COVID	Provost	Weibe			$20K	
UG	CoS Dean	Kirken		$9 K	$9K	
C Sharp Cook Endowed Professorship	Endowment	Pederson	Pederson		$300K	$100K
Schlumberger Foundation	Sabbatical Recruit	Dr. Winfred Mulwa	Pederson	$40K	$37K	
Naval Academy	Sabbatical Visitor	Dr. Daniel Finkenstadt	Pederson	$134K	$134K	
Faculty Endowment	Clare Luce Boothe Foundation	Dr. Gates and Ms. Keating	Pederson	$250K	$250K	
Total				$7.7M	$6.5M	$5.6M

Invited presentations since joining UTEP (2019-2024)

1. Nanoscale Molecular Magnets: Chemical Candidates for **Qubits and Quantum Sensors?** Mark R Pederson, Los Alamos National Laboratory (Fall 2019).
2. Molecular Magnets: Discovery from and Challenges for Electronic Structure **Mark R. Pederson**, A.I. Johnson, K. Dema, Z. Hooshmand, C. B. Shahi (US Africa Symposium on Electronic Structure, spring 2020).
3. Molecular Magnets: Chemical Models for Protons, Qubits, and Quantum Sensors? **Mark R. Pederson**
   (a) Ames Laboratory, (August, 2020)
   (b) University of Minnesota Department of Chemistry, (November 2020)
   (c) Temple University, (November 2021)
   (d) Rutgers Department of Physics (Decemeber 2021)
   (e) University of Texas - Austin (January 2022)
4. Undergraduate and Graduate Research in Physics: Vexing Challenges For Today, Opportunities for Tomorrow, **Mark R Pederson** (Tulane University 13 September 2021).
5. Quantum Now: Minimalist Methods for Quantum Calculations and Experiential Learning, Peter Lasode, Gustavo Bravo Flores, Christine Garcia, Ourania Glezokou, Vanda Glezokou, Ruben Ramos, Garry D. Woodruff and **Mark R Pederson** (Chicago, APS March Meeting 2021).
6. Symmetry Breaking and Restoration in Fermi-Lowdin-Orbital Self-Interaction Corrected Density Functional Approximations, **M.R. Pederson**, G. Bravo Flores ,K. Dema , K. Withanage, Z. Hooshmand , T. Baruah, K.A. Jackson, Computational Physics (August 2022).
7. Molecular Magnets: Models for Qubits, Quantum Sensors and Protons, A. I. Johnson, K. Dema, Z. Hooshmand, and **M. R. Pederson** MAGNA (Feb 2020).
8. MAGNA (December 2023)
9. Quantum Now: Minimalist Methods for Quantum Calculations and Experiential Learning, Peter Lasode, Gustavo Bravo Flores, Christine Garcia, Ourania Glezokou, Vanda Glezokou, Ruben Ramos, Garry D. Woodruff and **Mark R. Pederson** (Chicago, APS March Meeting 2021).
10. Nanoscale Molecular Magnets: Chemical Candidates for Qubits and Quantum Sensors? **Mark R. Pederson** (US Africa Symposium on Electronic Structure April 2022).
11. Self-Interaction Corrections to Density Functional Theory, Fall School on Correlated Materials, **Mark R Pederson** Forschungzentrum, Julich, Germany September 2023.
12. Self Interaction Corrections to Density Functional Theory: Applications to Molecular Magnets, 2nd-Annual US-North-Africa Meeting, (Spring 2022) **Mark R Pederson** (mrpederson@utep.edu)
13. Self Interaction Corrections to Density Functional Theory: Applications to Molecular Magnets, **Mark R Pederson** (Spetses, Greece July 2023).
14. Magneto-Electric Coupling, Chirality, and Symmetry Considerations in Molecular Spin Systems, **Mark R. Pederson**, Tunna Baruah, Fhokrul Islam and others. Interactional Symposium on Organic Metals, Superconductors and Magnets, (Anchorage, Alaska September 2024).
15. Improvements of Density Functional Theory, **Mark Pederson** The 2025 Meeting Joint meeting of the American Physical Society (Anaheim, CA March 2025).
16. Emergence of chirality in molecular magnets and frustrated molecular systems, **Mark R Pederson** (Spetses, Greece June 2025).

19 ISI publications and 1 book chapter at UTEP (since 2019)

1. *Theoretical studies of the vibrational properties of octahedrane (C12H12): A polyhedral caged hydrocarbon molecule* Finkenstadt, Daniel and Mehl, Michael J and **Pederson, Mark R** and Richardson, Steven L, The Journal of Chemical Physics **150** 21304 (2019).

2. *Magnetic Signatures of Hydroxyl-and Water-Terminated Neutral and Tetra-Anionic Mn12-Acetate* Batool, Javaria and Hahn, Torsten and **Pederson, Mark R**, Journal of Computational Chemistry **40** 2301-2308 (2019).

3. *A multiferroic molecular magnetic qubit*, Johnson, Alexander I and Islam, Fhokrul and Canali, Carlo M and **Pederson, Mark R**, The Journal of chemical physics **151** (2019).

4. *Electromagnetic control of spin ordered Mn 3 qubits: a density functional study* Hooshmand, Zahra and **Pederson, Mark R**, Physical Chemistry Chemical Physics **22** 27547-27553 (2020).

5. *Self-interaction correction in water–ion clusters* Wagle, Kamal and Santra, Biswajit and Bhattarai, Puskar and Shahi, Chandra and **Pederson, Mark R** and Jackson, Koblar A and Perdew, John P, The Journal of Chemical Physics **154** (2021).

6. *Electronic and magnetic signatures of low-lying spin-flip excitonic states of Mn12O12-acetate* Dema, Karma and Hooshmand, Zahra and **Pederson, Mark R**, Polyhedron **206** 115332 (2021).

7. *Initial Fermi orbital descriptors for FLOSIC calculations: The quick-FOD method* Nguyen, Duyen B and **Pederson, Mark R** and Perdew, John P and Jackson, Koblar A and Peralta, Juan E, Chemical Physics Letters **780** 138952 (2021).

8. *Electronic control of strong magnetic anisotropy in Co-based single-molecule magnets* Hooshmand, Zahra and Yu, Jie-Xiang and Cheng, Hai-Ping and **Pederson, Mark R**, Physical Review B **104** 134411 (2021).

9. *Complex Fermi–Löwdin orbital self-interaction correction* Withanage, Kushantha PK and Jackson, Koblar A and **Pederson, Mark R**, The Journal of Chemical Physics **156** 23110 (2022).

10. *Electric control of spin states in frustrated triangular molecular magnets* Nossa, JF and Islam, MF and **Pederson, Mark R** and Canali, Carlo M, Physical Review B **107** 245402 (2023)

11. *Density Matrix Implementation of the Fermi–Löwdin Orbital Self-Interaction Correction Method* Melo, Juan I and **Pederson, Mark R** and Peralta, Juan E, The Journal of Physical Chemistry A **127** 527–534 (2023).

12. *Downward quantum learning from element 118: Automated generation of Fermi–Löwdin orbitals for all atoms* **Pederson, Mark R** and Johnson, Alexander I and Withanage, Kushantha PK and Dolma, Sherab and Flores, Gustavo Bravo and Hooshmand, Zahra and Khandal, Kusal and Lasode, Peter O and Baruah, Tunna and Jackson, Koblar A, The Journal of Chemical Physics, **158** (2023).

13. *Comparative Density Functional Theory Study of Magnetic Exchange Couplings in Dinuclear Transition-Metal Complexes* Fitzhugh, Henry C and Furness, James W and **Pederson, Mark R** and Peralta, Juan E and Sun, Jianwei, Journal of Chemical Theory and Computation **19** 5760–5772 (2023).

14. *Room temperature colossal superparamagnetic order in aminoferrocene–graphene molecular magnets* Getahun, Yohannes W and Manciu, Felicia S and **Pederson, Mark R** and El-Gendy, Ahmed A, Applied Physics Letters **122** (2023).

15. *A perspective on sustainable computational chemistry software development and integration* Di Felice, Rosa and Mayes, Maricris L and Richard, Ryan M and Williams-Young, David B and Chan, Garnet Kin-Lic and de Jong, Wibe A and Govind, Niranjan and Head-Gordon, Martin and Hermes, Matthew R and Kowalski, Karol, **Pederson, Mark R** and others, Journal of Chemical Theory and Computation **19** 7056-7076 (2023).

16. *Use of FLOSIC for understanding anion-solvent interactions* **Pederson, Mark R** and Withanage, Kushantha PK and Hooshmand, Zahra and Johnson, Alex I and Baruah, Tunna and Yamamoto, Yoh and Zope, Rajendra R and Kao, Der-You and Shukla, Priyanka B and Johnson, J Karl and others, The Journal of Chemical Physics **159** (2023).

17. *Orbital dependent complications for close vs well-separated electrons in diradicals* Hooshmand, Zahra and Bravo Flores, Jose Gustavo and **Pederson, Mark R**, The Journal of Chemical Physics **159** (2023).

18. *Symmetry breaking and self-interaction correction in the chromium atom and dimer* Maniar, Rohan and Withanage, Kushantha PK and Shahi, Chandra and Kaplan, Aaron D and Perdew, John P and **Pederson, Mark R**, The Journal of Chemical Physics **160** (2024).

19. *Noncollinear first-principles studies of the spin-electric coupling in frustrated triangular molecular magnets* Islam, MF and Withanage, Kushantha PK and Canali, CM and **Pederson, Mark R**, Physical Review B **109** 214407 (2024).

20. **Self Interaction Corrections to Density Functional Theory**, Mark R. Pederson, va Pavarini and Erik Koch (eds.) Orbital Physics in Correlated Matter Modeling and Simulation, Vol. 13 Verlag des Forschungszentrum Jülich, 2023 ISBN 978-3-95806-689-2.

Some discipline-building activities and adventures throughout career

- Four Marathons: Twin Cities Marathon, Marine Corps Marathon (Twice), Washington Marathon.
- Chesapeake Bay Swim: 4.3 mile swim on what was the second or third most challenging day for this race in its forty year history. Very cold water with strong currents. I was amongst the 25 percent that finished (Everyone survived). Usually 80-95 percent of the starters finish.
- Biked from Munich to Budapest just before the wall fell.
- Visited Moscow immediately after the failed coup.
- Galapagos tour in a boat made for twelve.

Recognitions since coming to UTEP

2022,2023, 2024 — **Top two percent of scientists, internationally, in the field of Chemical Physics.**

2024 — **Most highly cited researcher at UTEP**

Research Publications from Direct ISI Web of Science Download (Slightly Abridged)

Journal Articles

1. E. J. Bylaska, A. Panyala, N. P. Bauman, *et al.*, "Electronic structure simulations in the cloud computing environment," *JOURNAL OF CHEMICAL PHYSICS*, vol. 161, no. 15, Oct. 2024. DOI: 10.1063/5.0226437.

2. M. F. Islam, K. P. K. Withanage, C. M. Canali, and M. R. Pederson, "Noncollinear first-principles studies of the spin-electric coupling in frustrated triangular molecular magnets," *PHYSICAL REVIEW B*, vol. 109, no. 21, Jun. 2024, ISSN: 2469-9950. DOI: 10.1103/PhysRevB.109.214407.

3. R. Maniar, K. P. K. Withanage, C. Shahi, A. D. Kaplan, J. P. Perdew, and M. R. Pederson, "Symmetry breaking and self-interaction correction in the chromium atom and dimer," *JOURNAL OF CHEMICAL PHYSICS*, vol. 160, no. 14, Apr. 2024, ISSN: 0021-9606. DOI: 10.1063/5.0180863.

4. R. Di Felice, M. L. Mayes, R. M. Richard, *et al.*, "A perspective on sustainable computational chemistry software development and integration," *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*, vol. 19, no. 20, pp. 7056–7076, Sep. 2023, ISSN: 1549-9618. DOI: 10.1021/acs.jctc.3c00419.

5. H. C. C. Fitzhugh, J. W. W. Furness, M. R. R. Pederson, J. E. E. Peralta, and J. Sun, "Comparative density functional theory study of magnetic exchange couplings in dinuclear transition-metal complexes," *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*, vol. 19, no. 17, pp. 5760–5772, Aug. 2023, ISSN: 1549-9618. DOI: 10.1021/acs.jctc.3c00336.

6. Y. W. Getahun, F. S. Manciu, M. R. Pederson, and A. A. El-Gendy, "Room temperature colossal superparamagnetic order in aminoferrocene-graphene molecular magnets," *APPLIED PHYSICS LETTERS*, vol. 122, no. 24, Jun. 2023, ISSN: 0003-6951. DOI: 10.1063/5.0153212.

7. Z. Hooshmand, J. G. Bravo Flores, and M. R. Pederson, "Orbital dependent complications for close vs well-separated electrons in diradicals," *JOURNAL OF CHEMICAL PHYSICS*, vol. 159, no. 23, Dec. 2023, ISSN: 0021-9606. DOI: 10.1063/5.0174061.

8. J. I. Melo, M. R. Pederson, and J. E. Peralta, "Density matrix implementation of the fermi-lo?wdin orbital self- interaction correction method," *JOURNAL OF PHYSICAL CHEMISTRY A*, vol. 127, no. 2, pp. 527–534, Jan. 2023, ISSN: 1089-5639. DOI: 10.1021/acs.jpca.2c07646.

9. J. I. Melo, M. R. Pederson, and J. E. Peralta, "Density matrix implementation of the fermi-lo?wdin orbital self-interaction correction method," *JOURNAL OF PHYSICAL CHEMISTRY A*, 2023 JAN 4 2023, ISSN: 1089-5639. DOI: 10.1021/acs.jpca.2c07646.

10. J. F. Nossa, M. F. Islam, M. R. Pederson, and C. M. Canali, "Electric control of spin states in frustrated triangular molecular magnets," *PHYSICAL REVIEW B*, vol. 107, no. 24, Jun. 2023, ISSN: 2469-9950. DOI: 10.1103/PhysRevB.107.245402.

11. M. R. Pederson, A. I. Johnson, K. P. K. Withanage, *et al.*, "Downward quantum learning from element 118: Automated generation of fermi-lowdin orbitals for all atoms," *JOURNAL OF CHEMICAL PHYSICS*, vol. 158, no. 8, Feb. 2023, ISSN: 0021-9606. DOI: 10.1063/5.0135089.

12. M. R. Pederson, K. P. K. Withanage, Z. Hooshmand, *et al.*, "Use of flosic for understanding anion-solvent interactions," *JOURNAL OF CHEMICAL PHYSICS*, vol. 159, no. 15, Oct. 2023, ISSN: 0021-9606. DOI: 10.1063/5.0172300.

13. C. Wilde, S. Memon, L. Ah-Kye, A. Milligan, M. Pederson, and H. Timlin, "A novel simulation model significantly improves confidence in canthotomy and cantholysis among ophthalmology and emergency medicine trainees," *JOURNAL OF EMERGENCY MEDICINE*, vol. 65, no. 5, e460–e466, Nov. 2023, ISSN: 0736-4679. DOI: 10.1016/j.jemermed.2023.05.009.

14. K. P. K. Withanage, K. A. Jackson, and M. R. Pederson, "Complex fermi-lowdin orbital self-interaction correction," *JOURNAL OF CHEMICAL PHYSICS*, vol. 156, no. 23, Jun. 2022, ISSN: 0021-9606. DOI: 10.1063/5.0091212.

15. K. Dema, Z. Hooshmand, and M. R. Pederson, "Electronic and magnetic signatures of low-lying spin-flip excitonic states of mn₁₂012-acetate," *POLYHEDRON*, vol. 206, Sep. 2021, ISSN: 0277-5387. DOI: 10.1016/j.poly.2021.115332.

16. Z. Hooshmand, J.-X. Yu, H.-P. Cheng, and M. R. Pederson, "Electronic control of strong magnetic anisotropy in co-based single-molecule magnets," *PHYSICAL REVIEW B*, vol. 104, no. 13, Oct. 2021, ISSN: 2469-9950. DOI: 10.1103/PhysRevB.104.134411.

17. D. B. Nguyen, M. R. Pederson, J. P. Perdew, K. A. Jackson, and J. E. Peralta, "Initial fermi orbital descriptors for flosic calculations: The quick-fod method," *CHEMICAL PHYSICS LETTERS*, vol. 780, Oct. 2021, ISSN: 0009-2614. DOI: 10.1016/j.cplett.2021.138952.

18. K. Wagle, B. Santra, P. Bhattarai, *et al.*, "Self-interaction correction in water-ion clusters," *JOURNAL OF CHEMICAL PHYSICS*, vol. 154, no. 9, Mar. 2021, ISSN: 0021-9606. DOI: 10.1063/5.0041620.

19. Z. Hooshmand and M. R. Pederson, "Electromagnetic control of spin ordered mn₃ qubits: A density functional study," *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*, vol. 22, no. 47, Dec. 2020, ISSN: 1463-9076. DOI: 10.1039/d0cp04455e.

20 J. Batool, T. Hahn, and M. R. Pederson, "Magnetic signatures of hydroxyl- and water-terminated neutral and tetra-anionic mn₁₂-acetate," *JOURNAL OF COMPUTATIONAL CHEMISTRY*, vol. 40, no. 26, pp. 2301–2308, Oct. 2019, ISSN: 0192-8651. DOI: 10.1002/jcc.26008.

21 D. Finkenstadt, M. J. Mehl, M. R. Pederson, and S. L. Richardson, "Theoretical studies of the vibrational properties of octahedrane (c₁₂h₁₂): A polyhedral caged hydrocarbon molecule," *JOURNAL OF CHEMICAL PHYSICS*, vol. 150, no. 21, Jun. 2019, ISSN: 0021-9606. DOI: 10.1063/1.5096404.

22 A. I. Johnson, F. Islam, C. M. Canali, and M. R. Pederson, "A multiferroic molecular magnetic qubit," *JOURNAL OF CHEMICAL PHYSICS*, vol. 151, no. 17, Nov. 2019, ISSN: 0021-9606. DOI: 10.1063/1.5127956.

23 T. Hahn, S. Schwalbe, J. Kortus, and M. R. Pederson, "Symmetry breaking within fermi-lowdin orbital self-interaction corrected density functional theory," *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*, vol. 13, no. 12, pp. 5823+, Dec. 2017, ISSN: 1549-9618. DOI: 10.1021/acs.jctc.7b00604.

24 M. A. Hosn, B. Adams, M. Pederson, T. Kresowik, and L. Pascarella, "Long-term effect of the type of carotid endarterectomy on blood pressure," *ANNALS OF VASCULAR SURGERY*, vol. 39, pp. 204–208, Feb. 2017, ISSN: 0890-5096. DOI: 10.1016/j.avsg.2016.05.129.

25 D.-y. Kao and M. R. Pederson, "Use of lowdin orthogonalised fermi orbitals for self-interaction corrections in an iron porphyrin," *MOLECULAR PHYSICS*, vol. 115, no. 5, SI, pp. 552–559, 2017, ISSN: 0026-8976. DOI: 10.1080/00268976.2016.1225992.

26 D.-y. Kao, M. R. Pederson, T. Hahn, T. Baruah, S. Liebing, and J. Kortus, "The role of self-interaction corrections, vibrations, and spin-orbit in determining the ground spin state in a simple heme," *MAGNETOCHEMISTRY*, vol. 3, no. 4, Dec. 2017. DOI: 10.3390/magnetochemistry3040031.

27 Z.-h. Yang, M. R. Pederson, and J. P. Perdew, "Full self-consistency in the fermi-orbital self-interaction correction," *PHYSICAL REVIEW A*, vol. 95, no. 5, May 2017, ISSN: 2469-9926. DOI: 10.1103/PhysRevA.95.052505.

28 M. Pederson, J. Cromwell, J. J. Mezhir, and P. Nau, "Sarcopenia is a predictor of surgical complications in a population younger than 40 years suffering from inflammatory bowel disease," *GASTROENTEROLOGY*, vol. 150, no. 4, 1, S1192–S1193, Apr. 2016, 57th Annual Meeting and Residents Fellow Conference of the Society-for-Surgery-of-the-Alimentary-Tract (SSAT) / 52nd Annual Meeting on Digestive Disease Week (DDW) / Meeting of the American-Gastroenterological-Association (AGA), San Diego, CA, MAY 21-24, 2016, ISSN: 0016-5085. DOI: 10.1016/S0016-5085(16)34031-8.

29 M. R. Pederson, T. Baruah, D.-y. Kao, and L. Basurto, "Self-interaction corrections applied to mg-porphyrin, c₆₀, and pentacene molecules," *JOURNAL OF CHEMICAL PHYSICS*, vol. 144, no. 16, Apr. 2016, ISSN: 0021-9606. DOI: 10.1063/1.4947042.

30 T. Hahn, S. Liebing, J. Kortus, and M. R. Pederson, "Fermi orbital self-interaction corrected electronic structure of molecules beyond local density approximation," *JOURNAL OF CHEMICAL PHYSICS*, vol. 143, no. 22, Dec. 2015, ISSN: 0021-9606. DOI: 10.1063/1.4936777.

31 M. R. Pederson, "Communication: Practical and rigorous reduction of the many-electron quantum mechanical coulomb problem to o(n^{2/3}) storage," *JOURNAL OF CHEMICAL PHYSICS*, vol. 142, no. 14, Apr. 2015, ISSN: 0021-9606. DOI: 10.1063/1.4917303.

32 M. R. Pederson, "Fermi orbital derivatives in self-interaction corrected density functional theory: Applications to closed shell atoms," *JOURNAL OF CHEMICAL PHYSICS*, vol. 142, no. 6, Feb. 2015, ISSN: 0021-9606. DOI: 10.1063/1.4907592.

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Books and Chapters

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  - Thesis: Orbital Dependent Improvements of DFT: Applications to Atoms, Molecules and Crystalline Silicon
- Naval Research Laboratory Materials Theory Postdoc 1986

Appointments

- Professor and Char, Physics, Univ of Texas at El Paso (2019-Present)
- Program Manager, Comp. and Theor. Chem., DOE (2008-2019)
- Research Professor, Chemistry, Johns Hopkins University (2013-2018)
- Researcher and Section Head, Naval Research Lab (1988-2008)
- Expert, Materials Sciences Division, NSF (2007-2008)
- Program Officer, Theoretical Chemistry, NSF (2002-2003)
- Sabbatical Max-Planck-Institute (Stuttgart) (1993-1994)

Ten Relevant Publications (234 Publications total)
(ISI: H-Index 52, >31000 Citations).

[1] ***Local-Density Hartree-Fock Theory of electronic states of molecules with self-interaction corrections***, MR Pederson, RA Heaton and CC Lin, J. Chem. Phys. **80** 1972 - 1975 (1984)**[119 Citations].**

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Synergistic Activities

(1) Primary developer of NRLMOL (DFT-based code for large molecules) **(2)** Visiting or adjunct professorships at Chemnitz Technical Institute (Germany), Central Michigan University, Linneaus, University of Maryland, and Linneaus University (Sweden). **(3)** Expertise with FORTRAN, MPI, UNIX, and massively-parallel computer platforms. **(4)** Navy representative for the ONR-Georgia Tech Molecular Design Institute. **(5)** Approximately 30 US Government Outstanding Performance awards including DOE-BES award for "*advice on a new national initiative*" (MGI). **(6)** APS executive board for DCOMP(2007-2010) **(7)** Organizer of workshop on *Computational Modeling of Magnetically Ordered Molecules and Electronic Nanoscale Transport of Spins* (The Como Moments) http://www.complexcomolake.it/thecomomoments/ **(8)** NRL Edison Pure Science Award (2004) **(9)** Fellow of the American Physics Society (1996): *For significantly enhancing the density-functional-based predictive power …by unique developments, implementations and applications of novel computational algorithms.* **(10)** University of Wisconsin Distinguished Alumni Award in Physics (2014).

Graduate and Postdoctoral Co-Advisees:

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OTHER PROFESSIONAL RECOGNITION, HIGHLIGTS AND RESPONSIBILITIES

•BES chemistry lead on two major computational science computing initiatives(Spring 2012)•BES Lead on approximately four research need studies (2008-2011)•BES SciDAC representative (2008-Present) • Advisory Board for NSF Teragrid (2010-Present)•BES Chemistry NERSC Allocation Manager (2008-

Present) •External Reviewer for Thesis Defense at Toulouse University (Candidate: R. Maurice (2011) •Short Term (20%) Detail Assignment at NSF DMR (2007-2008) •At Large Representative (Elected Position), APS Division of Computational Physics Executive Board (2007-2010)•Short Term (20%) Expert Detail Assignment at NSF DMR (2007-2008)•NRL Edison Pure Science Award 2004 • Research featured in Psi-K Feb 2004 "Scientific Highlight of the Month"•NSF Program Officer – Theoretical and Computational Chemistry 2002-2003 •Member of Advisory Board to the Georgia Tech Molecular Design Institute, 8/00-8/01. •Officer, NRL Sigma Xi Edison Chapter, 1999-2003. •NRL Contracting Officer Representive/Grant Monitor (1996-Present). •Editor of Book and Special Physica Status Solidi Volume entitled **Computer Modelling of Materials Properties and Phenomena**, PSSb **217**, Volume 1 (2000); •APS Fellow (Divison of Computational Physics) - 1999; •NRL Outstanding Performance Rating – Every Year while at NRL •Served on Illinois/Pittsburgh Supercomputing Peer Review Board 92-95; •Served on NSF Metacenter Review Board 92-95; •Highest Score on Univ. of Wisc. PhD Candidacy Exam Fall 83; •Reviewer for NSF, DOE, ONR, Swiss NSF, Israeli NSF, Ireland NSF, PRB, PRL, SSL, PSS, APL, JPC, JCP, CPL, PCCP, CTC , Nature Chemistry, Nature, Science, journals.

PROFESSIONAL POSITIONS

- 1978-1981 Undergraduate research at the University of Michigan – Ann Arbor (Physics).
- 1981-1986 Graduate Teaching & Research Assistantships University of Wisconsin Madison (Physics)
- 1986-2008 Postdoctoral, Staff, and Supervisory Theoretical Physics Researcher at the Naval Research Laboratory (Washington DC)
- 2008-2019 Program Manager at Department of Energy (Computation and Theoretical Chemistry)
- 2019-Present, Chair Department of Physics, University of Texas at El Paso

Professional position details:

a. Undergraduate researcher with Professor Bill Williams and Carl Wieman on Parity violation – theory and experiment (University of Michigan, 1979).

b. Undergraduate research with Professor Lawrence Sulak and Dr. Richard Bionta on the University of Michigan/Brookhaven Proton Decay Experiment (University of Michigan, 1980-1981).

c. Teaching Assistant in the University of Wisconsin Physics Department (1981-1982).

d. Research Assistant in the University of Wisconsin Physics Department (1982-1986).

e. National Research Council Rank-A Research Associate at the Naval Research Laboratory (1986-1988).

f. Physics Researcher in the Condensed-Matter and Radiation Sciences Division at the Naval Research Laboratory (1988-1995).

g. Sabbatical at Max-Planck-Institute fur Festkerporforschung (Solid State research) in Stuttgart Germany (1993-1994).

h. Member NSF Pittsburgh/Illinois Peer Review Board for Computer allocations (1993-1997).

i. Fellow of the American Physical Society (1999-Present).

j. Supervisory Theoretical Physicist in the "Clusters, Molecules, and Nanoscale Devices" Section at the Naval Research Laboratory (1996-2008).

k. Visiting Professor of Physics, Chemnitz Institute of Technology (Chemnitz Germany, Summer 1996).

l. Naval Researcher with cognizance over the ONR-Georgia-Tech Molecular Design Institute (1996-2001).

m. Courtesy Adjunct Professor at Central Michigan University Department of Physics (1995-1998).

n. Program Officer, National Science Foundation Theoretical and Computational Chemistry (2002-2003).

o. Executive Board of the American Physical Society Division of Computational Physics (2006-2009)

p. Advisory Board of the NSF Computing Centers (2009-2013).

q. Adjunct Visiting Scientist, Department of Chemistry, Johns Hopkins University (2004-2013).

r. Research Professor, Department of Chemistry, Johns Hopkins University (2013-Present).

s. Honorary appointment as Adjunct Professor of Chemistry, University of Maryland College Park (2004-2008).

t. Expert, National Science Foundation, Theoretical Condensed-Matter-Physics and Materials Science Program, (2008).

u. Program Manager in Computation and Theoretical Chemistry in the Department of Energy Office of Basic Energy Science (2008-Present).

v. Basic Energy Sciences Computer Allocations POC for Chemical Sciences (2008-Present)

w. Management Team for rollout of the DOE BES Energy-Frontier Research Centers (2009-2010).

x. External Dissertation Examiner (Lead) for Molecular Magnetism, University of Toulouse (2011).

y. External Dissertation Advisor, Department of Physics Linneaus University (Sweden) (2009-2013).

z. APS Division of Computational Physics Nominating Committee (2015 and Lead 2016).

aa. Advisory Committee to the Phase 1 (Lead) and Phase II University of Nebraska/University of Puerto Rico NSF Epscor Research Centers.\

TEACHING AND LECTURING EXPERIENCE

a. Classical Physics.
b. Classical Electricity and Magnetism
c. Undergraduate Research Laboratories.
d. Advanced Electronic Structure
e. Advanced Molecular Magnetism

ADMINISTRATIVE EXPERIENCE

a. NCSA-CMU/Pittsburgh Computer Allocation Committee (1993-1997)
b. NRL Contracting Officer Representive/Grant Monitor (1996-Present).
c. Supervisory Research Physicist Naval Research Laboratory (1998-2008).
d. Officer NRL Edison Chapter of Sigma Xi (1999-2003).
e. Program Officer, Theoretical and Computational Chemistry, National Science Foundation (2002-2003).
f. Expert, Theoretical Condensed Matter Physics and Materials Sciences, National Science Foundation (2008).
g. Executive Board of the American Physical Society Division of Computational Physics (2007-2010).
h. Program Manager, Computation and Theoretical Chemistry, Office of Basic Energy Sciences, Department of Energy (2008-Present).
i. Phase I (Lead) and Phase II advisory board to the University of Puerto Rico-University of Nebraska Center for Nanoscale Materials (2009-2011).
j. Lead on two Office of Science community reports on future of computational sciences (2011,2012).
k. Chemistry lead for the BES Exascale Science report (to be released in 2017).
l. Organizational Team for the BES Basic Research Needs Workshop on Catalysis (Spring 2017).
m. Panelist for various NSF and DOE review committees.

MEETINGS AND WORKSHOPS ORGANIZED

a. Focused Session for the March 2019 Meeting of the American Physical Society March Meeting (Division of Chemical Physics) *Molecular Magnets and Quantum Information* (March 2019).
b. International workshop on *Computational Modeling of Magnetically Ordered Molecules and Electronic Nanoscale Transport of Spins* (The Como Moments), Como, Italy (August 2013).
c. International Workshop on Theory of Atomic and Molecular Clusters, Richmond VA (May 2007).
d. CECAM Workshop on Models and Theory for Molecular Magnetism, Lyon France (July 2006).
e. 11^{th} and 12^{th} Annual International Materials Research Congress, Materials Design Using Molecular Simulation, Cancun Mexico (August 2002 and 2003).
f. Workshop on Massively Parallel and Superscalar Applications in Computational

Materials Science, Paderborn Germany (August 1998).

g. Workshop on Materials Physics, Chemnitz Germany (June 1996).
h. April American Physical Society Centennial Meeting, Division of Chemical Physics Symposium on Catalysis and Reactivity, Clusters and Nanoclusters, Atlanta GA (April 1996).
i. March American Physical Society Centennial Meeting, Division of Materials Physics Symposium on Clusters and Nanoclusters, Atlanta GA (March 1995).
j. August Meeting of the American Chemical Society, Diamond Chemical Vapor Deposition: Theory and Simulation, New York NY (August 1991).

SUPERVISORY EXPERIENCE

Postdoctoral Scholars (*de facto*): Prof. Koblar A Jackson, Prof. Andrew A Quong, Dr. David Patton, Dr. Dirk Porezag, Prof. Jens Kortus, Prof. Tunna Baruah, Prof. Kyungwha Park, Prof. Ben Powell, Dr. Reeshemah Allen, Dr. F. Islam, Dr. T. Hahn

Graduate Students (*de facto*): Dr. J.L. Chen (Maryland) Dr. D. Porezag (Chemitz, Germany), Dr. A. Sieck (Paderborn, Germany), Dr. C.H. Chien (George Mason University), Dr. C. Ashman (Virginia Commonwealth University), Dr. C. Schindelin (Bayreuth, Germany), K. Brake (Queensland, Australia), Prof. Jordi Ribas (Barcelona, Spain), Dr. F. J. Nossa (Linneaus University, Sweden), Dr. L. Michalak (Lineause University, Sweden), Dr. Alyson Butendyk (Johns Hopkins University, Sweden), Dr. Der-you Kao (George Washington University), Javaria Batool (Johns Hopkins University, Faisalbad Pakistan).

PRINCIPAL AREAS OF RESEARCH INTEREST

a. Density functional theory.
b. Self-Interaction Corrections to Density-functional theory.
c. Mathematical algorithms for electronic structure calculations.
d. Computational algorithms for electronic structure calculations.
e. Algorithms for massive parallel software.
f. NRLMOL
g. Diamond chemical vapor deposition.
h. Fullerene physics and chemistry.
i. Infrared and Raman spectra of molecules.
j. Excited electronic states.
k. Plasmon excitations.
l. Simplified relativity in quantum mechanics.
m. Molecular magnetism.
n. Single-electron transport.
o. Light-Harvesting.
p. Maybe batteries and fuel cells.
q. Water splitting.

AWARDS AND DISTINCTIONS

a. While at the Naval Research Laboratory, Dr. Pederson received commendations "in recognition of exceptional performance" ever year between 1989 and 2008.
b. Primary Architect of the massively parallel NRLMOL code for electronic structure calculations on molecules.
c. Highest Score PhD Candidacy Exam, Department of Physics (Fall 1983).
d. Rank A National Research Council Naval Research Laboratory Postdoctoral Associate (1986-1988).
e. NRL Review Award for "Buckminsterfullerene: Building Blocks for New Materials".
f. Advanced Naval Graduate Award for one-year sabbatical at the Max-Planck-Institute Stuttgart (1993-1994)
g. Contracting Officer Representative Certification (1997)
h. Fellow of the American Physical Society, Division of Computational Physics (1999).
i. Department of the Navy Technology Transfer Award (2001).
j. NRL Edison Pure Science Award (2004).
k. Research on molecular magnets featured in the Psi-K scientific highlight of the month (2004).
l. DOE performance award for program-manager-based "advice on a new national initiative" (MGI).
m. University of Wisconsin Distinguished Physics Alumni Award (2014).

GRANTS

Between 1996 and 2008, Pederson managed an internal competitive NRL funds totaling approximately $4M during the 12-year time span. He served on internal collaborative projects that brought in approximately $600K during this period as well. In addition, he served as the NRL/ONR lead/PI on the following externally funded projects:

a. NRL-NRC Postdoctoral position funded by National Academy of Sciences (1986-1988) ~$60K.
b. Simulation of Diamond Chemical Vapor Deposition (1989) ($50K, ONR).
c. NSF/DAAD US/German Exchange Program 1993-1996 ($19K).
d. NRL Host for DFG, DAAD, and other European-funded Visiting Former East-German Graduate Student Awards (1993-1998) ~$100K.
e. Advanced Naval Graduate Award for Sabbatical at Max-Planck-Institute Stuttgart (1993) ~ $85K.
f. ONR-Georgia-Tech Molecular Design Institute (1995-2000) $450K.
g. CHSSI-II Funding Army Research Laboratory (2002) $50K.
h. Sponsor for ONR-London and ONR-Global conference support programs (2002-Present) ~ $20K
i. Sponsor for ONR-London and ONR-Global short-term visiting science programs for K Brake, B. Powell, M. Beltran, T. Hahn (2002-Present) ~ $60K

j. While at the Naval Research Laboratory, Dr. Pederson received commendations “in recognition of exceptional performance” ever year between 1989 and 2008.
k. “Calculation of Magnetic Anisotropy Energies” (1999-2002) ~$150K.
l. NRL Lead on competitive ASEE postdoctoral fellowship for Dr. R. Allen ~$200K (2006-2008).
m. DARPA “Spectroscopic Sensing” ~$300K (2007-2011).
n. NSF, Equipment Grant, $600K (2020-2022)
o. DOE, FLOSIC Supplement $100K (2020-2021)
p. DOE, MMQM EFRC $130K (2021-2022)
q. DOE, FLOSIC Renewal $628K (2021-2024)
r. PNNL, LDRD. $100K (2022-2024)

LIST OF PUBLICATIONS

Web of Science: H Index 52, >234 Publications, >31000 Citations

1. **Local-Density Hartree-Fock Theory of Electronic States of Molecules with Self-Interaction Corrections**, M. R. Pederson, R. A Heaton, C. C. Lin, J. Chem. Phys. **80**, 1972 (1984).
2. **Density-Functional Theory with Self-Interaction Correction: application to the Lithium molecule** M. R. Pederson, R. A. Heaton and C. C. Lin, J. Chem. Phys. **82**, 2688 (1985).
3. **A New Density-Functional for Fractionally Occupied Orbital Systems**, R. A. Heaton, M. R. Pederson and C. C. Lin, J. Chem. Phys. **86**, 258 (1987).
4. **All-Electron Self-Consistent Variational Method for Wannier-Type Functions**, M. R. Pederson and C. C. Lin, Phys. Rev. B **35**, 2273 (1987).
5. **Localized and Canonical Atomic Orbitals in Self-Interaction Corrected Density-Functional Theory**, M. R. Pederson and C. C. Lin, J. Chem. Phys. **88**, 1807 (1988).
6. **Density-Functional Based Studies of Oxygen Vacancies in SiO_2**, M. R. Pederson, J. G. Harrison and B. M. Klein, Mat. Res. Soc. Symp. Proc. **105**, 229 (1988).
7. **Improved Theoretical Methods for Studies of Defects in Insulators: Application to the F Center in LiF**, M. R. Pederson and B. M. Klein, Phys. Rev. B, **37**, 10319 (1988).
8. **Simulated Annealing with Floating Gaussians: Hellmann-Feynman Forces without Corrections**, M. R. Pederson, B. M. Klein and J. Q. Broughton, Phys. Rev. B **38**, 3825 (1988).
9. **Alternative Paths to Total Energies and Forces in Many Atom Systems**, M. R. Pederson, *Proceedings of the Third International Conference on Supercomputing and Second World Supercomputing Exhibition*, Vol I, 179 (1988).
10. **Studies of C-H Radicals and their Behavior Near the Hydrogenated Diamond (111) Surface**, M. R. Pederson, K. A. Jackson and W. E. Pickett, in *Technology Update on Diamond Films*, Ed. by R.P.H. Chang, D. Nelson, and A. Hiraki, (Mat. Res. Soc., Pittsburgh, 1989).
11. **Applications of Simulated Annealing in Electronic Structure Studies of Metallic Clusters**, M. R. Pederson, M. J. Mehl, B. M. Klein and J. G. Harrison, in *Atomistic Simulation of Materials*, Ed. by V. Vitek and D. J. Srolovitz, (Plenum Publishing 1989).
12. **Studies of Large Lithium Clusters and Their Vacancies with Highly Optimized Localized Orbitals**, M. R. Pederson, J. G. Harrison and B. M. Klein, Mat. Res. Soc. Symp. Proc. **141**, 153 (1989).
13. **Theoretical Studies of Defects in Insulators Within the Framework of the Local Density Approximation**, M. R. Pederson and B. M. Klein, Materials Science Forum **37**, 199 (1989).

14. **Metallic State of the Free-Electron Gas Within the Self-Interaction-Corrected Local-Spin-Density Approximation**, M. R. Pederson, R. A. Heaton, J. G. Harrison and C. C. Lin, Phys. Rev. B **39**, 1581 (1989).
15. **Variational Mesh for Quantum-Mechanical Simulations**, M. R. Pederson and K. A. Jackson, Phys. Rev. B **41**, 7453 (1990).
16. **First-Principles, General Potential Local-Orbital Calculations for Bulk Crystals**, S. C. Erwin, M. R. Pederson, and W. E. Pickett, Phys. Rev. B. **41**, 10437 (1990).
17. **Donor Levels and Impurity Atom Relaxation in Nitrogen and Phosphorous Doped Diamond**, K. A. Jackson, M. R. Pederson, and J. G. Harrison, Phys. Rev. B **41**, 12641 (1990).
18. **Accurate Forces in a Local-Orbital Approach to the Local Density Approximation**, K. A. Jackson and M. R. Pederson, Phys. Rev. B **42**, 3276 (1990).
19. **Nitrogen and Phosphorous Impurities in Diamond**, K. A. Jackson, M. R. Pederson and J. G. Harrison, Proc. of the 1989 MRS Fall Meeting, (Materials Research Society, Pittsburgh PA, 1990).
20. **Adsorption of Hydrocarbon Radicals on the Hydrogenated Diamond Surface**, K. A. Jackson, M. R. Pederson and W. E. Pickett, Proc. of the 1990 MRS Spring Meeting, (Mat. Res. Soc., Pittsburgh PA, 1990).
21. **Forces and Geometrical Optimization in First-Principles Atomic Cluster Calculations**, K. A. Jackson, M. R. Pederson and S. C. Erwin, Proc. of the 1990 MRS Spring Meeting, (Mat. Res. Soc., Pittsburgh PA, 1990).
22. **Energetics and Geometries of Hydrocarbon Radicals on the Diamond Surface**, M. R. Pederson, K. A. Jackson, and W. E. Pickett, *Proc. of the 20th International Conference on the Physics of Semiconductors*, Thessaloniki, Greece, PTE LTD, 1990).
23. **GaAs Tight-Binding Hamiltonians**, J. Q. Broughton, D. Papaconstantopoulos, M. R. Pederson and D. Singh, *Proc. of the 20th International Conference on the Physics of Semiconductors*, Thessaloniki, Greece, PTE LTD, 1990).
24. **GaAs Tight-Binding Hamiltonians for use in Molecular Dynamics**, J. Q. Broughton, D. Papaconstantopoulos, M. R. Pederson and D. Singh, Proc. of the 1990 MRS Fall Meeting, (Materials Research Society, Pittsburgh PA, 1990).
25. **Accurate Intramolecular Forces within a Gaussian Orbital Local-Density Framework: Progress Towards Real Dynamics**, M. R. Pederson and K. A. Jackson, in *Density Functional Methods in Chemistry*, pp 231-245, Ed. by J. K. Labanowski and J. W. Andzelm. (1991).
26. **First-Principles Calculations of Defect-Induced lattice Relaxation in Ionic Systems**, K. A. Jackson, M. R. Pederson and B. M. Klein, Phys. Rev. B **43**, 2364 (1991).
27. **Pseuodo-energies for Simulations on Metallic Systems**, M. R. Pederson and K. A. Jackson, Phys. Rev. B **42**, 7312, (1991) [Brief Report].
28. **Applications of SIC-LSD to Atoms, Molecules and Solids**, M. R. Pederson, CCP9 Newsletter (1991).

29. **Theory of Magnetic and Structural Ordering in Iron Clusters**, J. L. Chen, C. S. Wang, K. A. Jackson and M. R. Pederson, Phys. Rev. B **44**, 6558 (1991) [Rapid Communication].
30. **Local-Density-Approximation-Based Simulation of Hydrocarbon Interactions with Applications to Diamond Chemical Vapor Deposition**, M. R. Pederson, K. A. Jackson and W. E. Pickett, Phys. Rev. B **44**, 3891 (1991).
31. **Theoretical Studies of the Diamond/Vapor Interface**, M. R. Pederson, *Proc. of the 2nd International Conference on the New Diamond Science and Technology*, (Materials Research Society, Pittsburgh 1991).
32. **Electronic Structure of Crystalline K_6C_{60}** , S. C. Erwin and M. R. Pederson, Phys. Rev. Lett. **67**, 1610 (1991).
33. **Energetics of Icosahedrally Twinned Rare Gas and Aluminum Clusters**, L. L. Boyer and M. R. Pederson, *Proceedings of the 1990 MRS Fall Meeting*, (Materials Research Society, Pittsburgh 1991).
34. **New Theoretical Model for the Diamond 1s Core Exciton**, K. A. Jackson and M. R. Pederson, Phys. Rev. Lett. **57**, 2521 (1991).
35. **Enhanced Stabilization of C_{60} Crystals though Doping**, M. R. Pederson, K. A. Jackson and L. L. Boyer, Phys. Rev. B **45**, 6919 (1992).
36. **Localization of Excess Electrons in Cubic Na_nCl_m Clusters**, J. L. Chen, C. S. Wang, K. A. Jackson and M. R. Pederson, Phys. Rev. B **45**, 1927 (1992) [Brief Report].
37. **Theoretical Electronic Structure Studies of Diamond: Surfaces Adsorbates, Defects and Heterointerfaces**, W. E. Pickett, M. R. Pederson, K. A. Jackson and S. C. Erwin, Mat. Sci. and Eng. **14**, 87 (1992).
38. **Theoretical Studies of Diamond Surface Chemistry and Diamond-Metal Interfaces**, W. E. Pickett, M. R. Pederson, K. A. Jackson and S. C. Erwin, In *Wide Bandgap Semiconductors*, ed. by T.D. Moustakas, J. I. Pankove, and Y. Hamakawa (Mat. Res. Soc. 1991), **242**, 3
39. **A First Principles Investigation of Aluminum Clusters: Geometries, Reactivities, Stabilities and Polarizabilities**, M. R. Pederson, *Physics and Chemistry of Finite Systems: From Clusters to Crystals*, Vol II, Ed. by P. Jena *et al*, (Kuwar Academic Publishers, 1992).
40. **Electronic Structure of Fullerenes: Isolated Molecules and Metal Doped Crystals**, M. R. Pederson, S. C. Erwin, W. E. Pickett, K. A. Jackson and A. A. Quong, *Physics and Chemistry of Finite Systems: From Clusters to Crystals*, Vol II, Ed. by P. Jena *et al*, (Kuwar Academic Publishers, 1992) p. 1323.
41. **Atoms, Molecules Solids and Surfaces: Applications of the Generalized Gradient Approximation for Exchange and Correlation**, J. P. Perdew, J. A. Chevary, S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh, and C. Fiolhais, Phys. Rev. B **46**, 6671 (1992).
42. **Charge States, Vibrational Modes and Polarizabilities of Isolated Fullerene Molecules**, M. R. Pederson and A. A. Quong, Phys. Rev. B **46**, 12906 (1992).
43. **Calculation of the Stability and Polarizability of Isolated Fullerene Molecules as a Function of Charge State**, A. A. Quong and M. R. Pederson, *Proceeding of the 1992 MRS Spring Meeting* (1992).

44. **Theoretical Investigations of Fluorinated and Hydrogenated Diamond (100) Films**, M. R. Pederson and W. E. Pickett, in *Novel Forms of Carbon*, MRS Proc. **270**, Ed. by C. L. Renschler, J. J. Pouch and D. M. Cox (Mat. Res. Soc., Pittsburgh 1992) pp 389-394.
45. **Theoretical Electronic Structure Studies of Diamond: Surfaces, Adsorbates, Defects and Heterointerfaces**, W. E. Pickett, M. R. Pederson, K. A. Jackson and S. C. Erwin, Mat. Sci. and Engin. **B14**, 87 (1992).
46. **Nanocapillarity in Fullerene Tubules**, M. R. Pederson and J. Q. Broughton, Phys. Rev. Lett. **69**, 2689 (1992).
47. **Density-Functional-Based Linear and Non-Linear Polarizabilities of Fullerene and Benzene Molecules**, A.A. Quong and M. R. Pederson, Phys. Rev. B **46**, 13584 (1992) [Rapid Communications].
48. **Hydrocarbon Clusters: Building Blocks for New Materials**, M. R. Pederson, K. A. Jackson, W. E. Pickett and B. M. Klein, in *On Clusters and Clustering*, Ed. by Peter Reynolds, Elsevior Science Publishers (1993).
49. **Covalent Container Compound: Empty, endohedral and exohedral C_{28} complexes**, M. R. Pederson and N. Laouini, Phys. Rev. B **48**, 2733 (1993).
50. **Electronic Structure of Superconducting Ba_6C_{60}**, S. C. Erwin and M. R. Pederson, Phys. Rev. B **47**, 14657 (1993) [Rapid Communications].
51. **First-Principles Determination of the Interatomic Force-Constant Tensor of the Fullerene Molecule**, A. A. Quong, M. R. Pederson and J. L. Feldman, Sol. Stat. Comm. **87**, 535 (1993).
52. **Multipole approach to orientational interactions in solid C_{60}** ,T. Yildirim, A. B. Harris, S. C. Erwin and M. R. Pederson, Phys. Rev. B **48**, 1888 (1993).
53. **Formation of self-arranging Mo Cubes**, A. S. Edelstein, F. H. Katz, G. M. Chow, E. I. Altman, R. J. Colton, M. R. Pederson, and M. J. Mehl, Sol. Stat. Comm. **86**, 323 (1993).
54. **Electronic Structure Investigations of siloxenic clusters and films**, M. R. Pederson, W. E. Pickett and S. C. Erwin, Phys. Rev. B **48**, 17556 (1993).
55. **Chemistry inside a Cage: Electronic States of Group-IV Endohedral Atoms in C_{28}**, K. Jackson, E. Kaxiras and M. R. Pederson, Phys. Rev. B **48**, 17556 (1993).
56. **Theoretical and Experimental Study of the Surface Structure of MgO (001)**, J. B. Zhou, Y. Li, C. Lu., D. Langreth, T. Gustafsson, P. Haeberle and M. R. Pederson Proc. of the ICSOS-V Conference (Shanghai, August 1993).
57. **Fullerene Molecules and Tubules: Polarizabilities, Vibrational Modes and Nanocapillarity**, M. R. Pederson, A. A. Quong, J. Q. Broughton, and J. L. Feldman, Comp. Mat. Sci. **2**, 1994 Elsevior.
58. **Charge Transfer Effects in $KNBO_3$ and Sodium**, L. L. Boyer, M. J. Mehl and M. R. Pederson, To appear.
59. **Electron-Phonon Coupling in A_3C_{60}: Contributions from Intermolecular Modes**, W. E. Pickett, D. A. Papaconstantopoulos, M. R. Pederson and S. C. Erwin, J. of Superconductivity, **1**, 651, (1994).
60. **Theoretical study of passivated small fullerenes $C_{24}X_4$ (X=N, P, As) and their isoelectronic equivalents $(BN)_{12}X_4$**, E. Kaxiras, K. Jackson and M. R. Pederson, Chem. Phys. Lett. **225**, 448 (1994).

61. **Bonding of Endohedral Atoms in Small Carbon Fullerenes**, K. Jackson, E. Kaxiras, and M. R. Pederson, J. of Phys. Chem. **98**, 7805 (1994).
62. **First-Principles Determination of the Polarizabilities of Carbon Tubules as a Function of Length**, A. A. Quong and M. R. Pederson, Proc. of the 1994 MRS Spring Meeting (MRS, Pittsburgh, 1994).
63. **Boron hydride analogs of fullerenes**, A. A. Quong, M. R. Pederson and J. Q. Broughton, Phys. Rev. B **50**, 4787 (1994).
64. **Fullerene Dimers: Electronic Structure, Cohesive Energy and Vibrational Modes**, M. R. Pederson and A. A. Quong, Phys. Rev. Lett. **74**, 2319 (1995).
65. **Modeling CVD Diamond with Density-Functional Theory**, W. E. Pickett, M. R. Pederson and B. N. Davidson, Nanotechnology **5**, 172-178 (1994).
66. **Covalent Carbon Compounds: From Diamond Crystallites to Fullerene-Assembled Polymers**, M. R. Pederson, To appear in *Fundamental Materials Sciences: I*, Series Editor M.F. Thorpe, ***Electronic Properties of Solids using Cluster Methods***, Ed. by T. A. Kaplan and S. D. Mahanti, Plenum Press, New York (1994).
67. **Density-Functional based determination of the CH_3-CH_4 hydrogen exchange reaction potential**, M. R. Pederson, Chem. Phys. Lett. **230**, 54 (1994).
68. **Energetics and Structure of Toroidal Forms of Carbon**, J. K. Johnson, B. N. Davidson, M. R. Pederson and J. Q. Broughton, Phys. Rev B **50**, 17575 (1994).
69. **Density-Functional Based Studies of Transition States and Barriers for Hydrogen Exchange and Abstraction Reactions**, D. Porezag and M. R. Pederson, J. Chem. Phys. **102** 23 (1995)
70. **Towards Cluster-Cluster Reaction Barriers within the Density-Functional Approximation**, D. V. Porezag and M. R. Pederson in *Clusters and Nanostructured Materials* pp. 307-318, Ed. by P. Jena and S.N. Behera, (Nova Science Publishers, New York 1996) .
71. **Structure, Stability and Vibrational Properties of Polymerized C_{60}**, D. Porezag, M. R. Pederson, Th. Frauenheim and Th. Kohler, Phys. Rev. B **52**, 14963 (1995).
72. **Vibrational Signatures of Diamond Surfaces** Th. Frauenheim, Th. Koeler, M. Sternberg, D. Porezag and M.R. Pederson, Thin Solid Films **272**, 314-330 (1995).
73. **Copper Adsorption on MgO Surfaces**, Y. Li, D. Langreth and M. R. Pederson, Phys. Rev. B **52**, 6067 (1995).
74. **Electronic and Vibrational Spectroscopy of Fullerene Based Systems**, M. R. Pederson, D. V. Porezag, J. Feldman, B. Davidson, A. A. Quong, Th. Kohler and Th. Frauenheim, (To appear in J. of Optical Engineering 1996).
75. **Raman and IR Intensities: A Density-Functional Study** D. V. Porezag and M. R. Pederson, Phys. Rev. B **54**, 7830 (1996).
76. **Electronic Properties of the Electride-type Molecule Li(9-crown-3)$_2$; Comparison of Hartree-Fock and Local Density Approximations**, R. Rencsok, K. A. Jackson, T. A. Kaplan, J. F. Harrison, and M. R. Pederson, Chem. Phys. Lett. **262**, 207 (1996).

77. **IR and Raman Spectroscopy within Density-Functional Theory** D. V. Porezag and M. R. Pederson, in *Proc. of the Int. Symp. on Atomistically Engineered Materials*, (World Scientific, Singapore 1996).
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209. **Fermi orbital self-interaction corrected electronic structure of molecules beyond local density approximation**, T. Hahn, S. Liebing, J. Kortus and M.R. Pederson, Submitted to J. Chem. Phys. http://arxiv.org/abs/1508.00745

210. **Self-interaction corrections applied to Mg-porphyrin, C60 and pentacene, M.R. Pederson, T. Baruah, D.Y. Kao and L. Basurto,** (To be submitted, November 2015)

211. **The Role of Self-Interaction Corrections, Vibrations and Spin-Orbit Interaction in determining the Ground-Spin State of the Fe(II) Porphyrin**, D.Y. Kao, M.R. Pederson, T. Hahn, T. Baruah, S. Liebling and J. Kortus, (To be submitted, November 2015).

212. **Paradox of Self-Interaction Correction: How can anything so right be so wrong,** J. P. Perdew, A. Ruzsinszky, J. Sun and M.R. Pederson, Advances in Atomic, Molecular and Optical Physics **64** 1-12 (2015).

213. **Electronic Transport as a Driver for Self-Interaction Corrected Methods**, A. Pertsova, C.M. Canali, M.R. Pederson, I. Rungger and S. Sanvito, Advances in Atomic, Molecular and Optical Physics **64** 29-64 (2015).

214.

215. **Self-Interaction Corrections Within the Fermi-Orbital-Based Formalism**, M.R. Pederson and T. Baruah, Advances in Atomic, Molecular and Optical Physics **64** 153-178 (2015).

216. **Self-interaction corrections applied to Mg-porphyrin, C60, and pentacene molecules**, MR Pederson, T Baruah, D Kao, L Basurto The Journal of Chemical Physics 144, 164117 (2016).

217. **Symmetry Breaking within Fermi–Löwdin Orbital Self-Interaction Corrected Density Functional Theory** T Hahn, S Schwalbe, J Kortus, MR Pederson, Journal of chemical theory and computation 13 (12), 5823-5828 ((2017)).

218. **The Role of Self-Interaction Corrections, Vibrations, and Spin-Orbit in Determining the Ground Spin State in a Simple Heme**, D Kao, MR Pederson, T Hahn, T Baruah, S Liebing, J Kortus Magnetochemistry 3 31 (2017).

219. **Full self-consistency in the Fermi-orbital self-interaction correction** Z Yang, MR Pederson, JP Perdew Physical Review A 95 052505 (2017).

220. **Use of Löwdin orthogonalised Fermi orbitals for self-interaction corrections in an iron porphyrin**, D Kao and MR Pederson, Molecular Physics 115, 552-559 (2017).

221. **Self-interaction corrections applied to Mg-porphyrin, C60, and pentacene molecules**, Pederson, Mark R, Baruah, Tunna, Kao, Der-you, Basurto, Luis, The Journal of chemical physics,**144**, 164117 (2016).

222. **Use of Löwdin orthogonalised Fermi orbitals for self-interaction corrections in an iron porphyrin**, Kao, Der-you, Pederson, Mark R, Molecular Physics,**115**, 552-559 (2017).

223. **Full self-consistency in the Fermi-orbital self-interaction correction**, Yang, Zeng-hui, Pederson, Mark R, Perdew, John P, Physical Review A,**95** 052505 (2017).

224. **The role of self-interaction corrections, vibrations, and spin-orbit in determining the ground spin state in a simple heme**, Kao, Der-you, Pederson, Mark R, Hahn, Torsten, Baruah, Tunna, Liebing, Simon, Kortus, Jens, Magnetochemistry **3**, 31 (2016).

225. **Symmetry Breaking within Fermi–Löwdin Orbital Self-Interaction Corrected Density Functional Theory**, Hahn, Torsten, Schwalbe, Sebastian, Kortus, Jens, Pederson, Mark R, Journal of chemical theory and computation,**13**, 5823-5828 (2017).

226. **Theoretical studies of the vibrational properties of octahedrane (C12H12): A polyhedral caged hydrocarbon molecule**, Finkenstadt, Daniel, Mehl, Michael J, Pederson, Mark R, Richardson, Steven L, The Journal of chemical physics,**150**, 214304 (2017).

227. **Magnetic Signatures of Hydroxyl-and Water-Terminated Neutral and Tetra-Anionic Mn12-Acetate**, Batool, Javaria, Hahn, Torsten, Pederson, Mark R Journal of computational chemistry,**40**, 2301-2308 (2019).

228. **A multiferroic molecular magnetic qubit**, Johnson, Alexander I, Islam, Fhokrul, Canali, Carlo M, Pederson, Mark R, The Journal of chemical physics,**151**, 174105 (2019).

229. **Electromagnetic control of spin ordered Mn 3 qubits: a density functional study**, Hooshmand, Zahra, Pederson, Mark R, Physical Chemistry Chemical Physics,**22**, 27547-27553, (2020).

230. **Self-interaction correction in water–ion clusters**, Wagle, Kamal, Santra, Biswajit, Bhattarai, Puskar, Shahi, Chandra, Pederson, Mark R, Jackson, Koblar A, Perdew, John P, The Journal of Chemical Physics,**154**, 094302 (2021).

231. **Electronic and magnetic signatures of low-lying spin-flip excitonic states of Mn12O12-acetate**, Dema, Karma, Hooshmand, Zahra, Pederson, Mark R Polyhedron,**206**,115332 (2021).

232. Z. Hooshmand, J.-X. Yu, H.-P. Cheng, and M. R. Pederson, **Electronic control of strong magnetic anisotropy in Co-based single-molecule magnets**, PHYSICAL REVIEW B 104 (2021).

233. **Initial Fermi orbital descriptors for FLOSIC calculations: The quick-FOD method**, Nguyen, Duyen B, Pederson, Mark R, Perdew, John P, Jackson, Koblar A, Peralta, Juan E, Chemical Physics Letters, **780**, 138952 (2021).

234. **Complex Fermi-Lowdin self-interaction correction**, KPK Withanage, KA Jackson, MR Pederson, Journal of Chemical Physics, **156**, 231103 (2022)

235. Z. Hooshmand, J. G. Bravo Flores, and M. R. Pederson, **Orbital dependent complications for close vs well-separated electrons in diradicals**, JOURNAL OF CHEMICAL PHYSICS 159 (2023).

236. M. R. Pederson, K. P. K. Withanage, Z. Hooshmand, A. I. Johnson, T. Baruah, Y. Yamamoto, R. R. Zope, D.-Y. Kao, P. B. Shukla, J. K. Johnson, J. E. Peralta, and K. A. Jackson, **Use of FLOSIC for understanding anion-solvent interactions**, JOURNAL OF CHEMICAL PHYSICS 159 (2023).

237. R. Di Felice, M. L. Mayes, R. M. Richard, D. B. Williams-Young, G. K.-L. Chan, W. A. de Jong, N. Govind, M. Head-Gordon, M. R. Hermes, K. Kowalski, X. Li, H. Lischka, K. T. Mueller, E. Mutlu, A. M. N. Niklasson, M. R. Pederson, B. Peng, R. Shepard, E. F. Valeev, M. van Schilfgaarde, B. Vlaisavljevich, T. L. Windus, S. S. Xantheas, X. Zhang, and P. M. Zimmer- man, **A Perspective on Sustainable Computational Chemistry Software Development and Integration**, JOURNAL OF CHEMICAL THEORY AND COMPUTATION 19, 7056–7076 (2023).

238. H. C. C. Fitzhugh, J. W. W. Furness, M. R. R. Pederson, J. E. E. Peralta, and J. Sun, **Comparative Density Functional Theory Study of Magnetic Exchange Couplings in Dinuclear Transition- Metal Complexes**, JOURNAL OF CHEMICAL THEORY AND COMPUTATION 19, 5760– 5772 (2023).

239. Y. W. Getahun, F. S. Manciu, M. R. Pederson, and A. A. El-Gendy, **Room temperature colossal superparamagnetic order in aminoferrocene-graphene molecular magnets**, APPLIED PHYSICS LETTERS 122 (2023).

240. J. F. Nossa, M. F. Islam, M. R. Pederson, and C. M. Canali, **Electric control of spin states in frustrated triangular molecular magnets**, PHYSICAL REVIEW B 107 (2023).

241. M. R. Pederson, A. I. Johnson, K. P. K. Withanage, S. Dolma, G. B. Flores, Z. Hooshmand, K. Khandal, P. O. Lasode, T. Baruah, and K. A. Jackson, **Downward quantum learning from element 118: Automated generation of Fermi-Lowdin orbitals for all atoms**, JOURNAL OF CHEMICAL PHYSICS 158 (2023).

242. J. I. Melo, M. R. Pederson, and J. E. Peralta, **Density Matrix Implementation of the Fermi-Loewdin Orbital Self- Interaction Correction Method**, JOURNAL OF PHYSICAL CHEMISTRY A 127, 527–534 (2023).

INVITED TALKS, COLLOQUIA, AND SEMINARS

1. SEMINAR
   Orbital Dependent Improvements of the Local-Density-Approximation, Naval Research Laboratory, Washington DC, May 1986 Mark R. Pederson.

2. SEMINAR
Quantum Molecular Dynamics: Improved Methods for Electronic Structure Calculations, Florida State University, Tallahasee FL, January 1988, Mark R. Pederson

3. TALK
Total Energies and Forces in Many Atom Systems via Quantum Molecular Dynamics, Third International Conference on Supercomputing, Boston, MA, May 1988, Mark R. Pederson

4. TALK
Theoretical Methods for Quantum-Mechanical Studies within a Local-Orbital Framework, Second Annual Workshop on Computational Condensed Matter Physics, Urbana IL, March 1989, Mark R. Pederson

5. SEMINAR
Cluster-Based Studies of the Condensed Phase Within a Localized Orbital Framework, ATT Bell Labs, Murray Hill, NJ, May 1989, Mark R. Pederson

6. SEMINAR
Studies of Diamond Chemical Vapor Deposition, Dept of Physics, Univ. of Alabama-Birmingham, Birmingham AL, October 1989, Mark R. Pederson

7. TALK
Theoretical Studies of Hydrocarbon Clusters, Lake Arrowhead Workshop on Clusters, Lake Arrowhead, CA, January 1990, Mark R. Pederson, K. A. Jackson, W. E. Pickett, and B. M. Klein.

8. SOCIETY TALK
GaAs Total Energy Tight Binding Hamiltonian for Use in Molecular Dynamics, MRS Spring Meeting, San Francisco, CA, April 1990, Jeremy Q. Broughton and Mark R. Pederson

9. SEMINAR
Accurate Intramolecular Forces Within a Gaussian-Orbital Framework and Applications of Density-Functional Approaches to Chemistry, Ohio State Supercomputing Center, Workshop on Density-Functional Methods for Chemistry, Columbus Ohio, May 1990, Mark R. Pederson and K. A. Jackson

10. TALK
Accurate Forces for Molecular Dynamical Simulations on Atomic Clusters, Third Annual Workshop on Computational Condensed Matter Physics, Ohio State University, May 1990, K. A. Jackson and Mark R. Pederson

11. SOCIETY TALK
GaAs Total-Energy Tight-Binding Hamiltonians for Use in Molecular Dynamics, Electrochemical Society Meeting, Montreal, May 1990, J. Q. Broughton and M. R. Pederson

12. TALK
Outstanding Questions for a Theoretical Understanding of Diamond Chemical Vapor Deposition, ONR-SDIO-IST Diamond Review, Boston MA, June 1990, Mark R. Pederson

13. TALK
Theoretical Studies of the Diamond/Vapor Interface, Second International Conference on the New Diamond Science and Technology, Washington DC, September 1990, M. R. Pederson

14. TALK
Theoretical Cluster Physics: From Hydrocarbons to Transition Metal Clusters, East Coast Cluster Symposium, Johns Hopkins University, Baltimore, MD, January 1991, K. A. Jackson and M. R. Pederson

15. SEMINAR
Theoretical Studies of Diamond Chemical Vapor Deposition, University of Exeter, United Kingdom, February 1991, M. R. Pederson

16. PLENARY TALK
Applications of SIC-LSD to Atoms, Molecules and Solids, Workshop on Many-Body Effects in Strongly Correlated Ground States, March 1991, Cambridge University, United Kingdom, M. R. Pederson

17. TALK
Theoretical Studes of Adsorbate Interactions Near the Diamond/Vapor Interface, Daresbury Laboratory, Daresbury UK, March 1991, Mark R. Pederson

18. TALK
Application of the Self-Interaction Correction to Clusters, Imperial College, London United Kingdom, March 1991, Mark R. Pederson

19. TALK
Theoretical Investigations of Metallic, Insulating, and Semiconducting Clusters,

Joint American-Japanese Workshop on Cluster Physics, University of Maryland, March 1991, Mark R. Pederson

20. TALK
A Local-Density-Based Description of Polarizabilities of Metallic Clusters, Second International Conference on Clusters, VA Commonwealth University, Richmond VA, October 1991, Mark R. Pederson

21. TALK
Applications of LCAO to Hydrocarbons, Diamond, Bucky Balls and Fullerene Tubules, Max Planck Institute - Stuttgart, October 1992, Mark R. Pederson

22. LECTURE
Fullerene Molecules and Tubules: Stability, Reactivity, and Polarizabilities, Workshop on Applications of Density-Functional Theory to Quantum Chemistry: A CCP9 Study Weekend, Daresbury National Laboratory, Daresbury UK, February 1993. Mark R. Pederson

23. TALK
Applications of LDA to Novel Forms of Carbon: Diamond CVD, hydrocarbon molecules, and fullerene molecules, Chemnitz Technical University, Chemnitz Germany, May 1993, Mark R. Pederson.

24. TALK
The Shape of Silicon Clusters, First International Symposium on the Theory of Molecules and Clusters (TAMC I), Leer Germany, June 1993, E. Kaxiras, K. A. Jackson and M. R. Pederson

25. TALK
Local Density Approximation for Clusters and Molecules, First International Symposium on the Theory of Molecules and Clusters (TAMC I), Leer Germany, June 1993, K. A. Jackson, E. Kaxiras, and M. R. Pederson

26. TALK
Molecular Carbon Clusters Workshop on Electronic Structure Methods, Ringberg Castle (MPI), Germany, September 1993, Mark R. Pederson

27. SOCIETY TALK
Clusters: Theory of Reactivity and Stability, March Meeting of the American Physical Society, Pittsburgh PA, March 1994, Mark R. Pederson

28. SEMINAR
How Bucky Balls Hold Hands, Department of Physics, State University of New York - Stony Brook, May 1994, Mark R. Pederson

29. TALK
Covalent Carbon Compounds: From Diamond Crystallites to Fullerene Assembled Polymers, Workshop on Clusters for Solid-State Investigations, Michigan State University, July 1994, Mark R. Pederson

30. SEMINAR
Reactivities within Density-Functional Theory, Department of Physics, Central Michigan University, September 1994, Mark R. Pederson

31. TALK
Towards a Density-Functional-Based Understanding of Cluster-Cluster Reaction Mechanisms, International Workshop on Clusters and Nanostructured Materials, Puri India, January 1995 Mark R. Pederson

32. TALK
Towards Cluster-Cluster Reaction Barriers within the Density-Functional Approximation: Hydrogen Exchange Reactions, M. R. Pederson, Sandia National Laboratory, March 1995.

33. SOCIETY TALK
Localized Representations for Efficient Studies of Materials Properties, 1995 June Meeting of the APS Computational Physics Division, Pittsburgh PA, Mark R. Pederson

34. SEMINAR
Local-Orbital-Based Density-Functional Calculations on Carbon Clusters Department of Physics, Jeonbuk National University, Korea, 3-July 1995, Mark R. Pederson

35. SEMINAR
Electronic Structure and Vibrational Modes of Isolated and Polymerized Fullerene Molecules, Department of Physics, Seoul National University, Korea, 26-June 1995, Mark R. Pederson

36. SOCIETY TALK
Vibrational and Electronic Spectroscopy of Fullerene-Based Systems, Mark R. Pederson SPIE 1995 International Symposium on Optical Science, Engineering and Instrumentation, San Diego, 10-July 1995.

37. TALK
Towards a Density-Functional-Based Description of Reaction Barriers, M. R. Pederson, University of California-Davis Electronic Structure Workshop, March 1995.

38. SEMINAR
Density-Functional Theory For Carbon Clusters, Mark R. Pederson, Georgetown University, September 1994.

39. SEMINAR
Clusters and Cluster Assembled Materials, Mark R. Pederson Virginia Commonwealth University, Richmond, 1-December 1995 (Postponed).

40. SEMINAR
Density-Functional Theory and LCAO for Cluster Dynamics, Mark R. Pederson, George Mason University, 23-October 1995.

41. SEMINAR
Cluster-Cluster Reactivities within DFT, Mark R. Pederson, Exxon Research Corporation, Annandale NJ February 1996.

42. LECTURE
Applications of Density-Functional Theory to Clusters and Cluster-Assembled Materials, M.R. Pederson, Max Planck Working Group, Dresden University June 1996.

43. TALK
First-Principles Calculations of Clusters and Assemblies: Methods and Applications, M. R. Pederson, Workshop on *First-Principles, tight-binding and empirical methods for materials simulation*, Chemnitz Germany, 26-June (1996).

44. TALK
Raman and Infrared Spectra for Large Clusters within Density Functional Theory, Physics Colloquium, Mark R. Pederson, Chemnitz Technical Institute, May (1996).

45. TALK
Raman and IR Spectroscopy within Density-Functional Theory, Mark R. Pederson Laussane Switzerland (1996).

46. PLENARY LECTURE
Applications of the Generalized Gradient Approximation to Density-Functional Theory, M. R. Pederson, International PSIK Network Conference, Schwaebisch Gmuend, Germany 17-21 September (1996). (Talk given by D.V. Porezag due to Family Illness).

47. TALK
Recent Applications of Problems Related to Molecular Design, Mark R. Pederson Georgia-Tech ONR Molecular Design Institute, 23-October 1996.

48. COLLOQUIUM
Density-Functional Theory as a Tool for Understanding Reactions and Catalysis, Mark R. Pederson Joint Colloquium at the University of Pittsburgh Department of Chemistry and Chemical Engineering, 24-October 1996.

49. COLLOQUIUM
Vibrational Spectra of Clusters within Density-Functional Theory, Mark R. Pederson Colloqium at the Virginia Commonwealth University Department of Physics, May (1997).

50. TALK
Infrared and Raman Spectra of Metallic, Insulating and Semiconducting Clusters, M. R. Pederson, World Materials Congress, Cancun Mexico (September 1997).

51. TALK
First-Principles Techniques for Studying Materials in Reactive Environments, M. R. Pederson, D. C. Patton and D. V. Porezag (Mardi Gras 1998) Baton Rouge Louisiana, 19-21 February (1998).

52. SEMINAR
Applications of NRLMOL to Clusters, Molecules and Assemblies, M. R. Pederson, George Mason University (February 1998).

53. TALK
Applications, Algorithms and Challenges for Computational Study of Clusters and Molecules, M. R. Pederson, University of California Davis Materials Theory Workshop, 20-22 March (1998).

54. LECTURE
An Assessment of GGA and LDA for Molecules M. R. Pederson, Aspen Workshop on Density-Functional Theory for Insulators, Aspen CO (June 1998).

55. TALK
Simulation of Transition Metal and Transition Metal Carbide Clusters, M. R. Pederson, INT Workshop on Atomic Clusters (8-July 1998).

56. TALK
Massively Parallel Version of NRLMOL, Mark R. Pederson, International Workshop on Computational Materials Science, Paderborn, Germany (28-August 1998).

57. SEMINAR
Density-Functional Based Calculations of Transition-Metal Carbide Clusters, M. R. Pederson, Max-Plank-Institute (Stuttgart), (7/8-September 1998).

58. LECTURE
Density-Functional-Based Investigations of Nanoscale Systems: Theory and Applications M.R. Pederson *The R.G. Herb Condensed Matter Seminar*, University of Wisconsin - Madison (18-February 1999).

59. TALK
Electronic Structure, Magnetic Ordering and Spin-Orbit Coupling in Molecular Scale Magnets, M.R. Pederson and S.N. Khanna, *Workshop on New Methods in Electronic Structure*, University of Illinois, Urbana, (21-24 May 1999).

60. TALK
Electronic Structure, Magnetic Ordering and Spin-Orbit Coupling in Molecular Scale Magnets, M.R. Pederson Rutgers University - Camden, Department of Chemistry, (10 June 1999).

61. SEMINAR
Prediction of Resonant-Field Strengths for Spin Tunneling in Molecular Scale Magnets, M.R. Pederson, Colloquium, Department of Physics, Virginia Commonwealth University (3 September 1999).

62. COLLOQUIUM
Simulation of Molecular Scale Magnets: Magnetic Ordering, Anisotropy Barriers and Spin Tunneling M.R. Pederson, Colloquium, Department of Physics, University of Missouri - Kansas City, (10 September 1999).

63. SEMINAR
Design and Optimization of Molecular Magnets, Department of Chemistry, Georgia Institute of Technology, Atlanta March 9 2000.

64. LECTURE
LCAO For Design of Molecular Materials, M.R. Pederson *Symposium in honor of Prof. Chun Lin's 70th Birthday*, Department of Physics, University of Oklahoma, 13-14 October 2000.

65. SEMINAR
Magnetic Molecules, M.R. Pederson Department of Physics, George Mason University, 30-March 2000.

66. SEMINAR
Magnetic Molecules: Spin Tunneling Barriers and Anisotropy Energies within DFT M. R. Pederson, □$_k$ 2000 Conference, Schwaebisch Gmund, Germany August (2000).

67. SEMINAR
Density-Functional-Based Simulation of Molecular Magnets, Mark R. Pederson, Dept. of Physics, Iowa State University, January 2000.

68. SEMINAR
NRLMOL: Algorithms and Applications, Mark R. Pederson, Wright Patterson Air Force Base, June 2000.

69. SEMINAR
Computational Design of Molecular Nanomagnets, Mark R. Pederson, Department of Physics, Case Western Reserve University 18 September 2000.

70. SEMINAR
Molecular Nanomagnets, Mark. R. Pederson, Department of Physics, State University of New York - Stoney Brook, 15-April 2001.

71. SEMINAR
DFT for Molecular Magnets: Fun for all ages, Mark R. Pederson, Department of Physics, Tulane University, Feb. 2001.

72. PLENARY LECTURE
Molecular Magnets within DFT, Tunnel Splittings and Magnetic Anisotropies, Mark R. Pederson, CECAM, France (July 2002).

73. PLENARY LECTURE
Density Functional Based Simulation of Molecular Magnets, Mark R. Pederson, Kavli Institute for Theoretical Physics, Santa Barbara (December 2002).

74. TALK
2^{nd} and 4^{th}-order anisotropies in Molecular Magnets, ESCM 2002, Georgetown University, July 2002.

75. TALK
Design and Simulation of Molecular Magnets, Mark R. Pederson, European MRS Meeting, Strasbourg France, June 2003.

76. SEMINAR
Electronic structure based Investigations of Molecular Magnets, Mark R. Pederson, CCNY, Department of Physics, May 2003.

77. PLENARY LECTURE
Design and Simulation of Molecular Magnetic Materials, Mark R. Pederson, Plenary Talk, XII'th Annual International Materials Research Congress, (Cancun MX) August 2003.

78. SEMINAR
DFT-Based Simulation of Molecular Magnets: Effects of Solvents, Exchange and Vibron, Mark. R. Pederson, Department of Physics, State University of New York, Stoneybrook (September 2003).

79. SEMINAR
DFT for Molecular Properties, Mark R. Pederson, Department of Chemistry, Johns Hopkins University, Fall 2003.

80. PLENARY LECTURE
Quantum-Chemical-Based Simulation of Molecular Magnets, Mark R. Pederson, Plenary Lecture, Conference on Current Trends in Computational Chemistry, Jackson MS November 2003.

81. TALK
Density-Functional-Based Simulation of Molecular Magnets, Mark R. Pederson, Aspen Institute for Physics, January 2004.

82. SEMINAR
Design and Simulation of Molecular Magnets, Mark R. Pederson, Department of Physics Colloquium, Virginia Commonwealth University Feb 6 2004.

83. SOCIETY TALK
Density Functional Theory of Molecular Magnets, Mark R. Pederson, 2004 March Meeting , Montreal Canada.

84. LECTURE
Density Functional Theory for Molecular Nanomagnets, Joint Colloquium for TUV-Dresden and Dresden Technical University Department of Physical Chemistry, Dresden Germany (May 2004).

85. SEMINAR
Density Functional Theory of Molecular Magnets, Condensed Matter Physics, Department of Physics, University of Delaware, September 2004.

86. SEMINAR
Theory of Molecular and Nanoscale Magnets, Mark R. Pederson, Department of Physics Colloquium, University of Florida – Gainesville, October 18 2004.

87. SEMINAR
Applications of NRLMOL to Nanoscience: From Molecular Magnets to Solar Harvesting, Mark R. Pederson, Chemical Physics, Department of Chemistry and Biochemistry, University of Maryland College Park (Feb 2 2005).

88. SEMINAR
Density Functional Theory for Design of Cluster-Based Materials, Mark R. Pederson, Department of Chemistry, University of Nebraska – Lincoln (February 22 2005).

89. SEMINAR
Density Functional Theory for Disordered Melanin-Based Conducting Polymers, Mark R. Pederson, University of Queensland, Australia (27 May 2005).

90. LECTURE
Theory and Computation of Molecular Magnetic Properties: Formalism, Numerics, Pitfalls, Solutions and Questions, M.R. Pederson, Summer School on Molecular Magnetism, ITP, Trieste Italy (27 June 2005).

91. SEMINAR
The role of polarization in a biomimetic photovoltaic molecule: A density-functional view point. (Greece, October 2005 ---Cancelled due to visa problems).

92. PLENARY LECTURE
Density-Functional Theory for Molecular Magnets, Wilhelm and Else Hereus Workshop on Molecular Magnetism, Germany (13-16 Nov 2005).

93. TALK
Applications of Density-Functional Theory to Molecular Magnets, Mark R. Pederson, ICCMSE, Key West FL (Fall 2005).

94. SEMINAR
Applications of Density-Functional Theory to Molecular Magnets,CECAM Lyon France (July 2006).

95. SEMINAR
The Role of Polarization in Materials Physics, Mark R. Pederson, Department of Physics, Virginia Commonwealth University, Richmond VA (September 2005).

96. SEMINAR
Density-Functional-Based Simulation of Light Harvesting in a Biomimetic Molecule, Department of Physics, Virginia Tech University, Blacksburg VA (12 Oct 2005).

97. JOINT CHEMISTRY AND PHYSICS SEMINAR
Density-Functional-Based Simulation of Molecular Magnets, Mark R. Pederson, Department of Physics, University of California Berkeley, 3-October 2005.

98. SEMINAR
The role of polarization in Materials Physics, Department of Physics, University of Missouri – Kansis City, 4-November 2005.

99. TALK
Simulation of Photoabsorption and Luminescence in Biomolecular Materials", Mark R. Pederson, International Materials Research Congress, Cancun MX (August 2006).

100. SEMINAR
Computational Design of Materials, Mark R. Pederson College-wide Seminar, The University of Akron, 12 October 2006.

101. COLLQUIUM
Density-functional-Based Simulation of Molecular Magnets and Light-Harvesting Molecules, Mark R. Pederson, Chemistry Colloquium (Johns Hopkins University, 17-April 2007).

102. TALK
Density-functional-based simulation of Molecular Magnets, Mark R. Pederson, Fifth International Workshop of the theory of atomic and molecular clusters (TAMCV), Richmond VA (May 2007).

103. PLENARY LECTURE
Massively Parallel Simulation of a Biomimetic Light-Harvesting Molecular Triad, Mark R. Pederson, Invited Plenary Talk, DoD HPCMO User Group Conference (Pittsburgh, June 2007).

104. COLLOQUIUM
Density-functional-Based Simulation of Molecular Magnets and Light-Harvesting Molecules, Mark R. Pederson, Colloquium (University of Puerto Rico – San Juan, 24-October 2007).

105. SEMINAR
Density-functional-based determination of Heisenberg Hamiltonians, Mark Pederson, Department of Physics, Virginia Commonwealth University, Richmond VA 16 November 2007.

106. TALK
Density-Functional-Based Simulation of Field-Induced Driving of Biomolecular Molecules, Mark R. Pederson, XI International Workshop on Complex Systems, Andalo Italy (15-20 March 2008).

107. TALK
Calculation of vdW interactions withing DFT, Mark R. Pederson Invited Talk, Spring MRS Meeting, San Francisco (25 March 2008).

108. TALK
Applications of a Massively Parallel Computational Methods to Molecular Nanomagnets, Mark R. Pederson, Ninth International Workshop on State of the Art in Scientific and Parallel Computing, Trondheim Norway (14-16 May 2008).

109. SEMINAR
The role of weak interactions in Biomimetic Photovoltaics and their connection to energy transfer, Mark R. Pederson, University of Ruhr, Germany (19-May 2008).

110. LECTURE
New opportunities for simulation within first-principles Methods, Mark R. Pederson, Deutshe Forshunggemeinschaft Scientific Colloquium on First-Principle-Methods, 21-23 May 2008.

111. LECTURE SERIES
DFT from A to Z, Mark R Pederson, Three Week Lecture Series, University of Puerto Rico San Juan (16-30 July 2008) – Cancelled due to new position in BES.

112. SEMINAR
Update on ZnO molecular wire DFT Calculations, SUNY-Stonybrook (2 October 2008).

113. SEMINAR
A DFT Tutorial, Mark R Pederson, University of Puerto Rico, (9 October 2008).

114. LECTURE
Molecular Magnetism, Mark R. Pederson, Aspen Center for Physics (Jan 2009).

118. SEMINAR
Chemical Compass for Avian Navigation: DFT Calculations, Mark R Pederson, University of Barcelona , Spain (Mark Pederson).

119. SEMINAR
Calculation of Kinetic Exchange and Magnetic Anisotropy Energies in Molecular Magnets, Mark R. Pederson, University of Tarragona, Spain (March 2009).

120. SEMINAR
Modeling Transport across Molecular Magnets, Mark R Pederson, University of South Florida, September 2010.

121. SEMINAR
Modeling Transport across Molecular Magnets, Mark R Pederson, Florida State University, December 2010.

122. SEMINAR
Modeling Transport across Molecular Magnets, Mark R Pederson, University of Houston, March 2011.

123. SEMINAR
Spin-Ordering in a Frustrated Cu_3 Spin System, Mark R Pederson, Virginia Commonwealth University September 2010.

124. TALK
DFT for molecular magnets, anisotropy, spin ordering and transport, Mark R Pederson, International Workshop: Progress and Future Challenges in Computational Materials Science, Bremen Germany, March 2011.

125. PLENARY
Computational Challenges for Wide-Spread Use of Self-Interaction-Corrections: A retrospective, Sponsored by Psi-K and the Daresbury CECAM, Chester England September 2011.

122. SEMINAR
Magnetic Anisotropies, Spin-Ordering and Transport in Nanomagnets, Sweden September 2011.

127. SEMINAR
DFT-based Simulation of Molecular Magnets, Mark R. Pederson, Department of Chemistry, University of Minnesota, April 16, 2012. Host: Connie Lu

128. SOCIETY TALK
DFT-based Modeling of Field Dependent Control and Response of Nanomagnetic Molecules, Mark R Pederson, APS March Meeting – Invited Talk W34.00002. March 1, 2012.

129. SOCIETY TALK
DFT-based simulation of quasi-classical magnetic behavior in molecular magnets, Mark R Pederson, ACS Meeting August 2012, Symposium on "Bridging the gap between quantum mechanical and classical behavior".

130. LECTURE
DFT-based Modeling of Field-Dependent Control and Response of Nanomagnetic Molecules, Mark R Pederson Bonn Germany (October 2012).

131. TALK
DFT-based Modeling of Field-Dependent Control and Response of Nanomagnetic Molecules, Mark R Pederson, Judipur India (March 2013).

132. TALK
DFT-based Molecules of Electron-, Spin- and Energy Transfer Processes in Large Molecular Systems, Mark R Pederson, Coma Ruga, Spain (July 2013).

133. COLLOQUIUM
DFT-based Molecules of Electron-, Spin- and Energy Transfer Processes in Large

Molecular Systems, Mark R Pederson, Johns Hopkins University, Department of Chemistry (15 September 2013).

134. SEMINAR
Control of Molecular Magnets with Fields and Electrons, Mark R. Pederson, Department of Chemistry Statistical Mechanics Seminar, University of California at Berkeley (25 October 2013).

135. SEMINAR
DFT-based Modeling of Transport Phenomena and Molecular Magnets, Department of Chemistry, Michigan State University (5 November 2013).

136. SEMINAR
Prospects for Self-Interaction Corrected Density Functional Theory with Unitary Invariance: Applications to Small Molecules, Mark. R. Pederson, University of Minnesota Theoretical Chemistry Center, February (2014).

137. PLENARY LECTURE
Self-Interaction Corrections with Unitary Invariance in DFT, "Theory Days: SIC Workshop", University of Toulouse, France November (2014).

138. TALK
Molecular Magnets: Success within DFT and Challenges for SIC, Biannual International Workshop on Electronic Structure, Institute for Theoretical Physics, Trieste, Italy January (2015).

139. SOCIETY TALK
Self-Interaction Correction to Density Functional Theory with Unitary Invariance, Mark R. Pederson, 2015 March ACS Meeting. (Phys)

140. SEMINAR
Self-Interaction Correction to Density Functional Theory with Unitary Invariance, Mark R Pederson, University of Southern California, March 2015.

141. SEMINAR
Molecular Magnets: Successes within DFT and Challenges for SIC, Mark R Pederson, University of California – Riverside, November 2015.

142. COLLOQUIUM
Molecular Magnets: Successes within DFT and Challenges for SIC, Mark R Pederson, College of William and Mary, November 2015.

143. PLENARY LECTURE
Why Computational Chemists Must Mind All Gaps, Mark R. Pederson, Banquet lecture at the 2015 Current Trends in Computational Chemistry, Jackson Mississippi, November 2015.

144. LECTURE
Self-Interaction Corrections: Past, Present and Future, Mark R. Pederson, Celebratory Symposium for John P. Perdew's John Scott Award, November 2015.

145. SEMINAR
Molecular Magnets: Successes within DFT and Challenges for SIC, Mark R Pederson, Hunter College Minisymposium on Electronic Structure, December 2016.

146. SEMINAR
Molecular Magnets: Successes within DFT and Challenges for SIC, Mark R. Pederson, PACIFICHEM, December 2015.

147. SOCIETY TALK
Fermi-Orbitals for Unitarily Invariant SIC, Mark R. Pederson, APS March Meeting (March 2016).

148. SOCIETY TALK
Applications of Fermi-Orbital-Based Self-Interaction Correction to Large Molecules, M.R. Pederson, D.Y. Kao, T. Baruah, T. Hahn, S. Liebling, and J. Kortus, ACS March Meeting (March 2016) (COMP).

149. TALK
Fermi-Orbitals for Unitarily Invariant SIC, Mark R. Pederson, Majorana Center for Physics, Erice, Sicily (July 2016).

150. SEMINAR

Fermi-Orbitals for Unitarily Invariant SIC, Mark R. Pederson, Fritz-Haber Institute (August 2016).

151. TALK

Fermi-Orbitals for Unitarily Invariant SIC, Mark R. Pederson, EMN International Workshop on Density-Functional Theory, Las Vegas NV (October 2016).

152. TALK

Ruedenberg-Edmiston and Fermi-Lowdin Orbitals – Then and Now, Mark R. Pederson, Sanibel Symposium in Honor of Klaus Ruedenberg, St. Simons Island, Georgia (February 2019).

153. SOCIETY TALK

Molecular Magnets (TBD), Mark R Pederson, 2018 Spring ACS Meeting (Orlando Florida)