Anil Kumar Kandalam

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Academic and Professional Appointments

- Professor (August 2022 – Present)
  Department of Physics & Engineering, **West Chester University**, West Chester, PA
- Adjunct Professor (June 2024 – Present)
  Department of Physics, **Michigan Technological University**, Houghton, MI
- Associate Professor (August 2017 – July 2022)
  Department of Physics & Engineering, **West Chester University**, West Chester, PA
- Assistant Department Chair (August 2017 – July 2020)
  Department of Physics & Engineering, **West Chester University**, West Chester, PA
- Assistant Professor (August 2012 – July 2017)
  Department of Physics & Engineering, **West Chester University**, West Chester, PA
- Assistant Professor (August 2008 – July 2012)
  Department of Physics, **McNeese State University**, Lake Charles, LA
- Collateral/Visiting Assistant Professor (August 2006 – August 2008)
  Department of Physics, **Virginia Commonwealth University**, Richmond, VA
- Postdoctoral Research Associate (November 2002 – July 2006)
  Department of Physics, **Virginia Commonwealth University,** Richmond, VA
- Research Assistant/Thesis Parts Participant (June 2000 – Aug. 2000; June 2001 – Aug. 2001)
  Chemistry/Materials Science Division, **Argonne National Laboratory**, Argonne, IL

Education

Michigan Technological University, Houghton, MI
Ph.D., Physics (October 2002)

University of Hyderabad, Hyderabad, India
M.Sc., Physics (May 1997)

Research Interests

- *Computational Modeling of Nanoclusters and Nanoparticles:* Electronic structure, magnetic, optical properties, and reactivity of bare, ligated, and supported nanoclusters and nanoparticles.
- *Cluster to Crystal:* Growth pattern of clusters towards bulk, identification of baby crystals.
- *Nano-Catalysis:* Reactivity studies of molecules and clusters with metal, metal-oxide, core-shell nanoparticles, and metal oxide thin films, focusing on nano-catalysis.
- *Nano-Bio Hybrid Systems:* Modeling the interaction of nanoparticles with DNA/RNA and other biomolecules.

Academic and Research Highlights

- Peer-reviewed Publications: **56**, Book Chapter: **1**, Conference Proceedings: **4**
- **H-index**: **31** (Google Scholar), **30** (ResearchGate), **29** (Web of Science), **28** (Scopus)
- **Citations: 2934** (Google Scholar), **2576** (ResearchGate), **2489** (Web of Science), **2426** (Scopus)
- **Co-Editor:** Proceedings of SPIE, Volume 10174, International Symposium on Clusters and Nanomaterials, ISBN: 9781510608412, March **2017**.
- Co-authored a paper that was selected as the "***2012 Editors' Choice***" by the Journal of Chemical Physics (JCP) editors, an AIP publication.
- **Co-editor of a Special Issue titled** "Nanomaterials in energy, health, and environment" **in the *Journal of Nanoparticle Research*** *(Springer)* **(2012).**
- Very Important Paper (**VIP**) in Angewandte Chemie Int. Ed. (**2010**).

Research Proposals and Grants

- ***External Proposals funded at WCUPA*** (**Total: $1,008,845)**:
  - **Co-PI** on S-STEM NSF proposal (**January 2021 – January 2027**): $999,085.51 for five years.
  - **Senior Personnel** on Keystone LSAMP NSF proposal (**October 2023**): $804,107.64 for five years. **(Canceled in Spring 2025 during NSF refocusing)**.
  - **PI:** WCU Foundation FaStR grant (**January 2015**): $9760.00 for 1 year.

- ***Internal Competitive Proposals funded at WCUPA***:
  - WCU-COURSE Program; Co-PI (Fall 2019): $2000.00
  - University Research Funding (July 2016): $7162.00
  - College of Arts and Sciences Student Engagement Grant (June 2014): $7790.00
  - College of Arts and Sciences Support and Development Award (Dec 2013): $3000.00
- ***External Proposals Funded at McNeese***: BOR-RCS grant; Co-PI: $105,741.00

Teaching Experience

1. **Department of Physics & Engineering, West Chester University (2012 – present)**
   Courses taught to Physics majors:
   Physics I (PHY170), Physics II (PHY180), Modern Physics (PHY240), Electricity & Magnetism – I (PHY430), Quantum Physics – I (PHY420), Solid State Physics (PHY480), Introduction to Nanomaterials (PHY481), Quantum Mechanics – II (PHY425), Introduction to Nanoscience (PHY480).
   ***Courses taught to non-majors* (*General Education Courses*):**
   Elements of Physical Science (PHY 100), General Physics – I & II (PHY130 & PHY 140)

2. **Department of Physics, McNeese State University** (**2008 – 2012**)
   Upper-level courses taught to Physics majors:
   Modern Physics-I (PHYS341), Thermodynamics (PHYS421)
   Electricity and Magnetism-I and II (PHYS401 and PHYS402), Quantum Physics-I (PHYS481)
   Graduate/Undergraduate level multi-disciplinary courses taught:
   Nanoscience: Special Problems in Physics (PHYS441/CHEM526)

***Courses taught to non-majors* (*General Education Courses*):**
Physical Science-I (PHSC101), General Physics-I and II (PHYS201, PHYS202), University Physics-I (PHYS211)

3. **Department of Physics, Virginia Commonwealth University (2006 – 2008)**
Upper-level courses taught to Physics Majors:
Statistical Mechanics and Thermodynamics (PHYS340), Quantum Physics-I (PHYS380)
Graduate-level multi-disciplinary courses (Physics, Chemistry, and Engineering):
Structure and Bonding: From Atoms to Bulk: Topics in Physics (PHYS591)

Teaching Initiatives

- Designed, developed, and taught a CAPC-approved "**Science at the Nanoscale**" (**NSC201**) course in Spring 2025 for STEM majors.
- Designed, developed, and taught a new special-topics course, "**Introduction to Nanoscience**" **(PHY480)**, in Spring 2023 for 4th-year Physics majors.
- Designed and taught a CAPC-approved **Quantum Mechanics II (PHY425)** course in Spring 2022 for physics seniors.
- Designed, developed, and taught the lecture portion of a new CAPC-approved special topics course, "**Introduction to Nanomaterials**" **(PHY481)**, in Spring 2020 for 4th-year Physics majors.
- Developed and taught a special-topics course, "**Solid State Physics**" (PHY480), in Spring 2017 for 3rd- and 4th-year Physics majors.
- Designed, co-developed, and team-taught a new special-topics course, "**Nanoscience***,"* for Physics, Chemistry, and Engineering majors at McNeese State University.
- Designed, co-developed, and team-taught a special-topics course, "**Structure and Bonding: From Atoms to Bulk***,"* at VCU in Fall 2006

Scholarly and Professional Activities

- **Co-Organizer:** International Symposium on Clusters and Nanomaterials (ISCAN), Richmond, VA, Oct. 26 – 29, **2015**
- **Organizer:** 5th Jekyll Island Conference on Clusters and Nanostructures, Jekyll Island, GA, April 21 – 25, **2013**
- **Co-Organizer:** International Symposium on Clusters and Nanostructures (ISCAN), Richmond, VA, Nov. 7 – 11, **2011**
- **Co-Organizer:** 4th Jekyll Island Conference on Clusters, Jekyll Island, GA, Feb. 16-19, **2010**
- **Co-Editor:** Materials Issues in a Hydrogen Economy, Proceedings of the International Symposium, World Scientific Publications, Singapore, ISBN: 13 978-981-283-801-8, **2009**
- **Member of the Organizing Committee:** International Symposium on Materials Issues in a Hydrogen Economy, Richmond, VA, Nov 12-15, **2007**
- **Reviewer for Journals:** Journal of Chemical Physics, Physical Review B, Chemical Physics Letters, Journal of Physical Chemistry B and A, Journal of Physical Chemistry (*Letters*), Inorganic Chemistry, Physics Letters A, PCCP, and Journal of Nanoparticle Research

Research Presentations (Invited)

1. "*Stability, Magnetic, and electronic properties of gas-phase and supported MnO clusters*"
   Department of Physics & Astronomy, Villanova University, Villanova, PA, Oct 23, **2026**
2. "*Interaction of dopamine and DNA nucleobases with size-selected gold nanoclusters* **(poster)**"
   Gordon Research Conference (Clusters & Nanostructures), Mount Holyoke, MA, July 9 – 14, **2017**
3. "*Aluminum Zintl anions in gas-phase clusters*"
   Department of Physics, Indiana University of PA, Indiana, PA, April 7, **2017**
4. "*Aluminum Zintl anions in gas-phase clusters*"
   Department of Physics, Michigan Technological University, Houghton, MI, Sept. 15, **2016**
5. *"From Clusters to Crystals: A Bottom-Up Design"*
   International Symposium on Clusters and Nanomaterials (ISCAN), Richmond, VA, October **2015**
6. "*Feasibility of Aluminum Zintl anions in gas-phase clusters*"
   Department of Physics & Astronomy, Villanova University, Villanova, PA, Nov 14, **2014**
7. "*Electronic Structure and Growth Pattern of Aluminum Hydride Clusters: Emergence of bulk-like Structures.*"
   Department of Chemistry, Johns Hopkins University, Baltimore, MD, July 18, **2014**
8. "*Structural evolution of Lead Sulfide: from cuboids to baby crystal*"
   5th Jekyll Island Conference on Clusters and Nanostructures, Jekyll Island, GA, April **2013**
9. "*Growth pattern and emergence of bulk-like structure in Aluminum hydride clusters*"
   Southwest Regional American Chemical Society (ACS) meeting, Baton Rouge, Nov 5, **2012**
10. "*Unusual properties of $Au_n(BO_2)_m$ clusters: From Superhalogens to Hyperhalogens*"
    4th Jekyll Island Conference on Clusters and Nanostructures, Jekyll Island, GA, Feb **2010**
11. "*Probing the interaction between nanostructures and biomolecules: A computational investigation.*"
    Indo-US Workshop on Nanotechnology: Applications and Implications, Indian Institute of Chemical Technology (IICT), Hyderabad, India, Nov 10-12, **2009**
12. "*Hydrogen Storage in Materials*"
    International Workshop on Computational Materials Science, American University in Cairo, Egypt, Nov 17-20, **2008**
13. "*Nanomaterials with Novel Properties: A Theoretical Perspective*"
    Physics Department, University of Louisiana, Lafayette, LA Nov 6, **2008**
14. "*Clusters as Hydrogen Storage Compounds: Promise and Challenges*"
    Gordon Research Conference (Clusters, Nanocrystals & Nanostructures), Mount Holyoke, MA July 29 – Aug 3, **2007**
15. "*Novel Geometries and Electronic Properties of Organometallic Complexes and their Applications*"
    The International Workshop on Clusters, Jekyll Island, Georgia, Dec. 16-20, **2006**
16. "*Theoretical Investigation of CO Oxidation on Fe_2O_3 (0001) and (100) surfaces*"
    7th Philip Morris USA Symposium on Fundamental Science, Richmond, VA, Feb **2006**

17. "*Unique Magnetic Signature of Transition Metal Atoms on Organic Template*"
Dow Corning Corporation, Midland, MI, September **2003**

Hot-Topic Talks at International Conferences

- "*International Symposium on Clusters and Nanomaterials (ISCAN)*," Richmond, VA, October **2015**
- *"XV International Symposium on Small Particles & Inorganic Clusters (ISSPIC XV),"* Oaxaca, Mexico, September **2010**

Other Research Talks at Conferences

- *Neurotransmitter-conjugated Au-Ag bimetallic nanoclusters: Interaction of Au_xAg_y (x+y = 8 & 10) clusters with dopamine*
  Materials Research Society (MRS) Meeting, Symposium: Nanomaterials and Devices by Cluster Beam Deposition, Phoenix, AZ, April **2018**
- *Stability and Magnetic Coupling between Mn-doped Stannaspherenes*
  American Physical Society (APS) March Meeting; New Orleans, LA, March **2008**
- *Oxidation of CO in various Fe_2O_3 surfaces: A Theoretical Study*
  American Physical Society (APS) March Meeting; Baltimore, MD, March **2006**
- *Electron Counting rules for the stability of metal-encapsulated Si_n Cages*
  American Physical Society (APS) March Meeting; Los Angeles, CA, March **2005**
- *Geometry and Electronic Structure of $V_n(Benzene)_m$ complexes*
  American Physical Society (APS) March Meeting; Austin, TX, March **2003**

Research Supervision of Students

- The number of undergraduate/graduate students supervised in research since 2012: **14**.
- The number of high school students supervised in research since 2012: **4**.

Service to the Scientific Discipline

1. **Reviewer for *NRC – Research Associateship Program (RAP)*** applications administered by the Office of Fellowships at the National Academies (NAS). [**March 2025, May 2025, & Aug 2025, and May 2026 review cycles; 25 applications**]
2. ***Member***, PhD dissertation committee of a graduate student in the Physics Department at Michigan Technological University (Since Summer 2025)
3. **Reviewer:** *J. Chem. Phys.*, *PCCP, Phys. Rev. B, Chem. Phys. Lett., J. Phys. Chem. B & A, J. Phys. Chem. Lett., Inorg. Chem., and J. Nanoparticle Research.*
4. *External evaluator of a PhD Thesis* (Central University of Punjab, India, **2025**).
5. *External evaluator of a PhD Thesis* (Pune University, India, **2022**).

University Service at WCU

1. University Representative, *PASSHE FPDC Committee* (AY 2023 – 24 & 2024 – 25)
2. Founding Director, *WCU Center for Nanomaterials* (Fall 2020 – Fall 2023)
3. Reviewer, *PASSHE FPDC Annual Grant Program* (Spring 2019, Spring 2024)

4. Reviewer, *Provost Research Grants (PRG) Review Committee* (Fall 2018, Fall 2019, Fall 2020, Fall 2022, Fall 2023, Fall 2024)
5. Judge Poster presentations at *WCU Research and Creative Activity Day* (Fall 2019)
6. Co-President: *WCU Chapter of Sigma Xi*, the Scientific Research Honor Society (Spring 2019 – 2021).
7. Member, Search Committee to hire *Grants Development Specialist*, WCU Research and Sponsored Programs (Spring 2019)
8. Member, *Research and Creative Activity Advisory Board (RCAAB)* (Fall 2018 – present)
9. Judge, Poster presentations at *WCU Research and Creative Activity Day* (Fall 2018)
10. Member, APSCUF representative on the Search Committee for *Vice Provost for Research and Creative Activity* (AY 2017 – 2018)
11. Member, *Provost Research Grants (PRG) Evaluation Committee*, AY 2017 – 18 (Spring 2018)
12. Judge, Oral presentations at *WCU Research Day* (in Fall 2017)

College Service at WCU

1. Member, *Department Evaluation Committee of a BME faculty member* (AY 2026 – 27)
2. Member, *CMS Associate Dean Search Committee* (AY 2025 – 26)
3. Member, *5th-year evaluation committee of BME faculty member* (Zhongping Huang, AY 24-25)
4. Member, *CSM Celebrates!* CSM Research Day (Spring 2021)
5. Member, *CSM Undergraduate and Graduate Student Research Committee* (Fall 2019, Spring 2020, Spring 2021, Fall 2021)
6. Member, *RIMS Review Committee* (Fall 2018)
7. Member, *CSM Poster Session Coordination Committee* (Spring 2017, 2018)
8. Member, *College of Arts and Sciences (CAS) Recruitment Committee* (2012 – 2014)

Department Service at WCU

1. Member, *Tenure-track Faculty Search Committee* (AY 2026)
2. Member, *Department Evaluation Committee for promotion to Professor* (AY 25 – 26, Morrison)
3. Chair, *Department 5th-year Evaluation Committee of a Professor* (AY25 – 26, Mitchell)
4. Member, *Department Promotion Recommendation Committee for promotion to Professor* (AY 25 – 26, Waite)
5. Chair, *Department 5th-year Evaluation Committee of a Professor* (AY24 – 25, Aptowicz)
6. Member, *Department Evaluation Committee for promotion to Professor* (AY24 – 25, Chen)
7. Member, *Department Evaluation Committee for promotion to Professor* (AY 24 – 25, Waite)
8. Faculty Advisor, *Society of Physics Students (SPS)* (Fall 2022 – Summer 2025)
9. Chair, *Department Promotion Recommendation Committee for promotion to Professor* (AY23 – 24, Pfeil)
10. Chair, *Department Evaluation Committee of an Adjunct Faculty* (AY 23 – 24, Chyba)
11. Member, *Department Evaluation Committee of an Adjunct Faculty* (AY 23 – 24, Sawyer)
12. Chair, *Department 5th-year Evaluation Committee of a Professor* (AY22 – 23, Thornton)

13. Member, *Department Evaluation Committee for promotion to Professor* (AY22 – 23, Pfeil)

14. Member, *Department Promotion Recommendation Committee for promotion to Professor* (Fall 2022, Mitchell)

15. Member, *Department Curriculum Committee* (Fall 2015 – Spring 2021)

16. Chair, *Department Evaluation Committee of a tenure-track faculty member* (AY17 – 19)

17. Member, *Department Evaluation Committee of a tenure-track Faculty Member* (AY17 – 19)

18. Member, *Department Promotion Recommendation Committee for promotion to Professor* (Fall 2017, Thornton)

19. Member, *Hiring Committee/Search Committee for the department's AA position* (Spring 2018)

20. Chair, *Tenure-track Faculty Search Committee* (AY 2015 – 2016) to recruit two faculty members.

21. Member, *Tenure-track Faculty Search Committee* (AY 2013 – 2014)

22. Faculty Advisor, *Society of Physics Students (SPS)* (2012 – 2017)

RESEARCH PUBLICATIONS

(Student authors are denoted in blue color)

A. BOOK CHAPTER

"*Growth pattern and size-dependent properties of lead-chalcogenide nanoclusters*"
Ann F. Gill, William H. Sawyer, Kamron Salavitabar, B. Kiran, and Anil K. Kandalam**
"Clusters: Structure, Bonding, and Reactivity" Book Series: Challenges and Advances in Computational Chemistry and Physics, Volume: 23, Pages: 289 – 323, ISBN: 978-3-319-48918-6 (**2017**)

B. PUBLICATIONS IN JOURNALS

1. *Density functional theory study of the structure, stability, magnetic properties, and (hyper)polarizability of (sub-nm) rare-earth (RE) doped gold clusters: Au_5RE with RE = Sc, Y, La – Lu.*
   Mukesh Jakhar, Anil K. Kandalam**, Ravindra Pandey, B. Kiran, and Shashi P. Karna
   J. Chem. Phys. 160, 144306 (**2024**)

2. *Trapping of H_2^- in aluminum hydride, $Al_4H_{14}^-$*
   B. Kiran, K. H. Bowen, and A. K. Kandalam**
   J. Chem. Phys. (*Communication*): 155, 121101 (**2021**)

3. *A Combined Theoretical and Photoelectron Spectroscopy Study of $Al_3H_n^-$ (n = 1 – 9) clusters*
   J. Xu, X. Zhang, H. Wang, L. Fu, X. Li, A. Grubisic, R. M. Harris, B. Eichhorn, G. Gantefor, Y. Ding, B. Kiran, A. K. Kandalam, and K. H. Bowen
   Zeitschrift fur anorganische und allgemeine Chemie (*Z. anorg. allg. Chem.)*
   647 (18), 1840 – 1848 (**2021**)

4. *Ligated Aluminum Cluster Anions, LAl_n^- (n = 1-14, L = $N[Si(Me)_3]_2$)*
   G. Liu, S. M. Ciborowski, G. R. Montone, W. H. Sawyer, B. Kiran, Anil K. Kandalam**, and Kit H. Bowen
   Phys. Chem. Chem. Phys. 23, 15209 – 15215 (**2021**)

5. *Low Oxidation State Aluminum-containing cluster anions: $LAlH^-$ and LAl_n^- (n = 2 – 4, L = $N[Si(Me)_3]_2$)*
   X. Zhang, L. Wang, Georgia R. Montone, Ann F. Gill, G. Gantefor, B. Eichhorn, Anil K. Kandalam**, and K. H. Bowen
   Phys. Chem. Chem. Phys. 19, 15541 – 15548 (**2017**)

6. *Low Oxidation State Aluminum-containing cluster anions: $Cp^*Al_nH^-$, n = 1 – 3*
   X. Zhang, G. Gantefor, B. Eichhorn, D. Mayo, W. H. Sawyer, A. F. Gill, A. K. Kandalam**, H. Schnöckel, and K. H. Bowen
   J. Chem. Phys. 145, 074305 (**2016**)

7. *Superhalogens beget superhalogens: A case study with $(BO_2)_n$ Oligomers*
   Anil K. Kandalam**, B. Kiran, P. Jena, S. Pietsch, and G. Gantefoer
   Phys. Chem. Chem. Phys. (*Communication*) 17, 26589 (**2015**)

8. *Photoelectron Spectrum of a Polycyclic Aromatic Nitrogen Heterocyclic Anion: Quinoline*
A. M. Buytendyk, Y. Wang, J. D. Graham, A. K. Kandalam, B. Kiran, and K. H. Bowen
Molecular Physics 113, 15 – 16, 2095 (**2015**)

9. *Identification of hyperhalogens in $Ag_n(BO_2)_m$ (n = 1 – 3, m = 1 – 2) clusters: anion photoelectron spectroscopy and density functional calculations*
X. – Y. Kong, H. – G. Xu, P. Koirala, W. Zheng, A. K. Kandalam**, and P. Jena
Phys. Chem. Chem. Phys. 16, 26067 (**2014**)

10. *Photoelectron Spectroscopy of Boron Aluminum Hydride Cluster Anions*
H. Wang, X. Zhang, Y. J. Ko, G. F. Gantefoer, K. H. Bowen, X. Li, B. Kiran, and A. K. Kandalam
J. Chem. Phys. 140, 164317 (**2014**)

11. *The Viability of Aluminum Zintl Anion Moieties within Magnesium-Aluminum Clusters*
H. Wang, Y. J. Ko, X. Zhang, G. Gantafoer, H. Schnoeckel, B. Eichhorn, P. Jena, B. Kiran, A. K. Kandalam**, and K. H. Bowen
J. Chem. Phys. 140, 124309 (**2014**)

12. *Aluminum Zintl anion moieties within Sodium Aluminum Clusters*
H. Wang, X. Zhang, Y. J. Ko, A. Grubisic, X. Li, G. Gantefoer, H. Schnoeckel, B. Eichhorn, M. – S. Lee, P. Jena, A. K. Kandalam**, B. Kiran, and K. H. Bowen
J. Chem. Phys. 140, 054301 (**2014**)

13. *Electron tunneling characteristics of cubic quantum dot, $(PbS)_{32}$*
S. K. Gupta, H. He, D. Banyai, Anil K. Kandalam, and R. Pandey
J. Chem. Phys. 139, 244307 (**2013**)

14. *Anomalous Property of $Ag(BO_2)_2$ Hyperhalogen: Does Spin-Orbit Coupling Matter?*
H. Chen, Y. Kong, W. Zheng, J. Yao, Anil K. Kandalam, and P. Jena
ChemPhysChem 14, 3303 (**2013**)

15. *Electronic and Magnetic Properties of Manganese and Iron atoms decorated with BO_2 superhalogens*
P. Koirala, K. Pradhan, Anil K. Kandalam**, and P. Jena
J. Phys. Chem. A 117 (6), 1310 (**2013**)

16. *Origin of the anomalous magnetic behavior of Fe_{13}^+ cluster*
M. Wu, G. Gutsev, Anil K. Kandalam, and P. Jena
Phys. Rev. B. 86, 174410 (**2012**)

17. *Al_6H_{18}: A baby crystal of γ-AlH_3*
B. Kiran, Anil K. Kandalam**, J. Xu, Y. H. Ding, M. Sierka, K. H. Bowen, and H. Schnockel
J. Chem. Phys. 137, 134303 (**2012**)

18. *$(PbS)_{32}$: A baby crystal*
B. Kiran, Anil K. Kandalam, R. Rallabandi, P. Koirala, G. Gantefoer, X. Li, X. Tang, Y. Wang, H. Fairbrother and K. H. Bowen
J. Chem. Phys. 136, 024317 (**2012**)
(***Virtual Journal of Nanoscale Science & Technology***, Vol. 25, Issue 4, 2012)

19. *Superhalogen Properties of Cu_mCl_n Clusters: Theory and Experiment*
Y. J. Ko, H. Wang, K. Pradhan, P. Koirala, Anil K. Kandalam**, K. H. Bowen, and P. Jena
J. Chem. Phys. 135, 244312 (**2011**)

20. *Photoelectron Spectroscopic Studies of Iron–Pyrene Cluster Anions*
X. Li, K. H. Bowen, P. Jena, and Anil K. Kandalam**
J. Chem. Phys. 135, 204301 (**2011**)

21. *Structural Evolution and Stabilities of Neutral and Anionic Clusters of Lead Sulfide: Joint Anion Photoelectron and Computational Studies*
P. Koirala, B. Kiran, Anil K. Kandalam**, C. A. Fancher, H. L. de Clercq, X. Li, and K. H. Bowen
J. Chem. Phys. 135, 134311 (**2011**)

22. *Structures and Photoelectron Spectroscopy of $Cu_n(BO_2)_m^-$ (n,m = 1-2) Clusters: Observation of Hyperhalogen Behavior*
Y. Feng, H. G. Xu, W. Zheng, H. Zhao, Anil K. Kandalam**, and P. Jena
J. Chem. Phys. 134, 094309 **(2011)**

23. *Manganese-based Magnetic Superhalogens*
M. M. Wu, H. Wang, Y. J. Ko, Q. Wang, Q. Sun, B. Kiran, Anil K. Kandalam, K. H. Bowen Jr., and P. Jena
Angew. Chem. Int. Ed. (*Comm.*) 50, 2568 **(2011)**

24. *Hyperhalogens: Discovery of a new class of highly electronegative species*
M. Willis, M. Gotz, Anil K. Kandalam**, G. F. Gantefoer, and P. Jena
Angew. Chem. Int. Ed. (*Comm.*) 49, 8966 **(2010) (*VIP paper*)**

25. *Superhalogen properties of Fluorinated Coinage Metal Clusters*
P. Koirala, M. Willis, B. Kiran, Anil K. Kandalam, and P. Jena
J. Phys. Chem. C 114, 16018 **(2010)**

26. *Chain and Double-ring Polymeric Structures: Observation of $Al_nH_{3n+1}^-$(n=4-8) and $Al_4H_{14}^-$*
X. Li, A. Grubisic, K. H. Bowen, Anil K. Kandalam**, B. Kiran, G. F. Gantefoer, and P. Jena
J. Chem. Phys. (*Communication*), 132, 241103 **(2010)**

27. *Origin of the unusual properties of $Au_n(BO_2)$ Clusters*
M. Gotz, M. Willis, Anil K. Kandalam**, G. F. Gantefoer, and P. Jena
ChemPhysChem 11, 853 **(2010)**

28. *Reactivity of Neutral and Charged B_{13} Clusters with O_2: A Theoretical Study*
William J. Slough, Anil K. Kandalam, and R. Pandey
J. Chem. Phys. 132, 104304 **(2010)**

29. *Origin of the unusual stability of B_{12} and B_{13}^+ Clusters*
B. Kiran, G. G. Kumar, M. T. Nguyen, A. K. Kandalam, and P. Jena
InOrg. Chem. (*Communication*) 48 (21), 9965 **(2009)**

30. *Unique Magnetic coupling between Mn-doped Stannaspherenes ($Mn@Sn_{12}$)*
Anil K. Kandalam**,** G. Chen, and P. Jena
Appl. Phys. Lett. 92, 143109 (**2008**)

31. *Photoelectron Spectroscopy and Theoretical Studies of $[Co_m(pyrene)_n]$ (m, n = 1-2) Complexes*
Anil K. Kandalam**, P. Jena, X. Li, S. N. Eustis, and K. H. Bowen
J. Chem. Phys. 129, 134308 (**2008**)

32. *Photoelectron Spectroscopic Study of the Anionic Transition Metal-Organic Complexes, $[Fe_{1,2}(COT)]^-$ and $[Co(COT)]^-$*
X.Li, S. N. Eustis, K. H. Bowen, and Anil K. Kandalam*
J. Chem. Phys. 129, 124312 (**2008**)

33. *Photoelectron Spectroscopic Study of Iron-Benzene Cluster Anions*
W. Zheng, S. N. Eustis, X. Li, J. M. Nilles, O. C. Thomas, K. H. Bowen, and A. K. Kandalam*
Chem. Phys. Lett. 462, 35 (**2008**)

34. *The Photoelectron Spectroscopic and Theoretical Studies of $Fe_m(Coronene)_n^-$ (m = 1-2, n = 1-2) Complexes*
X. Li, S. Eustis, K. H. Bowen, Anil K. Kandalam**, and P. Jena
J. Chem. Phys. 129, 074313 (**2008**)

35. *Multi-Decker Organometallic Complexes as Hydrogen Storage Materials*
Anil K. Kandalam, B. Kiran, and P. Jena
J. Phys. Chem. C 112, 6181 (**2008**)

36. *Oxidation of CO on Fe_2O_3 Model Surfaces*
Anil K. Kandalam**,** B. Chatterjee, S. N. Khanna, B. K. Rao, P. Jena, and B. V. Reddy **Surface Science** 601, 4873 (**2007**)

37. *Ground state structures and Photoelectron spectroscopy of $[Co_n$-(Coronene)$]^-$ Complexes*
Anil K. Kandalam, B. Kiran, P. Jena, X. Li, A. Grubisic, and K. H. Bowen
J. Chem. Phys. 126, 084306 (**2007**)

38. *Hydrogen Storage and the 18-electron rule*
B. Kiran, Anil K. Kandalam, and P. Jena
J. Chem. Phys. 124, 224703 (**2006**)

39. *Structure and Bonding of Au_5M (M = Na, Mg, Al, Si, P, and S) Clusters*
C. Majumder, Anil K. Kandalam, and P. Jena
Phys. Rev. B 74, 205437 (**2006**)
(*Virtual Journal of Nanoscale Science & Technology,* Vol. 14, Issue 24, 2006**)**

40. *Effect of Au coating on the magnetic and structural properties of Fe nano-clusters for use in biomedical applications: A density-functional theory study*
Q. Sun, Anil K. Kandalam, Q. Wang, P. Jena, Y. Kawazoe, and M. Marquez
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*Only author of the theory part; **Corresponding author of the theory part

C. CONFERENCE PROCEEDINGS

1. *Interaction of size-selected gold nanoclusters with dopamine*
G. Montone, E. Herrmann, and A. K. Kandalam
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2. *Size-Selected Clusters on Surfaces*
X. Tang, X. Li, Y. Wang, K. Wepasnick, A. Lim, D. H. Fairbrother, K. H. Bowen, T. Mangler, S. Noessner, C. Wolke, M. Grossmann, A. Koop, G. Gantefoer, B. Kiran, and A. K. Kandalam
Journal of Physics: Conference Series 438, 012005 (**2013**)

3. *Metal-Benzene Complexes with Inserted Metal Atoms and the Possibility of Generating Magnetic Ni-Benzene Clusters*
Anil K. Kandalam, N. O. Jones, S. N. Khanna, and P. Jena,
Clusters and Nano-Assemblies: Physical and Biological Systems, Page: 341, World Scientific, Singapore (**2005**)
[Proceedings of International Symposium on Clusters and Nano-Assemblies (ISCANA), 2003]

4. *Prediction of Reduction Potentials with Quantum Chemical Methods*
N. J. Pennington, J. M. Vollmer, A. K. Kandalam, P. Zapol, L. A. Curtiss, C. Chen, D. R. Vissers, and K. Amine
Batteries and Capacitors (Electrochemical Society Series), Page: 389 – 394 (**2003**)
[Proceedings of International Symposium on Batteries and Supercapacitors, 2001]

D. MANUSCRIPTS UNDER PREPARATION/REVIEW

1. *Electronic and Optical Signatures of Lanthanide-Benzene Complexes across the 4f series*
N. S. Palaparambil, A. K. Kandalam, R. Pandey, and S. P. Karna
Materials Advances (**under review: 2026**)

2. *Magnetic nanocages: A DFT study of $(MnO)_n$ (n = 1 – 12, 14, and 16) nanoclusters.*

Thomas Whoriskey, Sriya Jonnadula, Matthew M. Waite, B. Kiran, and A. K. Kandalam. (*in preparation*: **2026**)

3. *Interaction of size-selected Au_n (n = 8, 10, and 20) nanoclusters with Dopamine*
   G. Montone, E. Herrmann, Matthew M. Waite, B. Kiran, and A. K. Kandalam (*in preparation*: **2026**)

Research in News

- "***$(PbS)_{32}$: A baby crystal***", published in the *Journal of Chemical Physics,* was selected as "**2012 Editor's Choice**" by the editors of JCP.
  - The American Institute of Physics (AIP) selected it to feature in their Physics News Highlights newsletter (01/17/2012): http://www.aip.org/aip/research/PNH-1-17-2012.html. The journal also chose it as a research highlight and featured it on the journal website home page (http://jcp.aip.org/jcp/).
  - It also appeared on several Science news websites, such as: EurekAlert!, the website operated by AAAS, "PhysOrg", "newswise.com", and "Physnews.com".
- "***Manganese based Magnetic Superhalogens***," published in *Angew. Chem. Int. Ed.* has appeared on several science news websites, such as:
  - "Science Daily," "Science Newsline," Breaking News on "EurekAlert!", "Institute of Nanotechnology (," "PhysOrg," "Laboratory Journal" (Wiley Publications), "ASM International," and "Scientific Computing."
  - It was also featured under "***Hot topics in Magnetic Materials***" by **Wiley Interscience**
- "***Hyperhalogens: Discovery of a New Class of Electronegative Species***," published in *Angew. Chem. Int. Ed.* has appeared on several science news websites. A few of them are:
  - October 18, 2010, issue of **C&EN**, the ACS weekly magazine, under "Science and Technology Concentrates" (Page 27)
  - ChemViews Magazine (www.chemistryviews.org), the online magazine of ChemPubSoc Europe (an organization of 16 European Chemical Societies).
  - "ASM International", The Materials Information Society
  - ***Breaking News*** on the "EurekAlert!" website operated by **AAAS**
  - Nanoscience and Technology Institute (NSTI), Institute of Nanotechnology (www.nano.org.uk), "Science Newsline," "PhysOrg," "Science Daily," and "Nanotech Wire."
- "***Origin of the unusual properties of $Au_n(BO_2)$ clusters***", published in ChemPhysChem 11, 853 (2010), was featured under "***Hot topics in Gold***" by **Wiley InterScience**.