DENIZ CAKIR, PhD

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Educational Background

August 2008 ***Ph.D.*, Physics (Computational condensed matter physics)**
Title of the thesis: "Titanium Dioxide Nanostructures for Photocatalytic and Photovoltaic Applications"
Bilkent University, Physics Department, Ankara/Turkey
Advisor: Prof. Dr. Oğuz Gülseren

August 2003 ***M.Sc.*, Physics**
Title of the thesis: Mechanical and Electronic Properties of Metal Chain Nanowires
University of Bilkent, Physics Department, Ankara/Turkey
Advisor: Prof. Dr. Oğuz Gülseren

June 2001 ***B.S.*, Physics**
Title of the senior project: Modulation field effect transistor
Middle East Technical University, Physics Department, Ankara/Turkey
Advisor: Prof. Dr. Mehmet Tomak

Professional Experience

08/21-present **Director's Fellowship of Materials and Manufacturing Initiative**, University of North Dakota

08/19-present **Adjunct Faculty**, Department of Chemistry, University of North Dakota

08/16-present **Assistant Professor of Physics**, Department of Physics and Astrophysics, University of North Dakota

07/13-08/16 **Post-Doctoral Research Associate**, Condensed Matter Theory Group, University of Antwerp, Belgium
- **Advisor:** Prof. Dr. Francois M. Peeters

09/12-07/13 **Visiting Researcher,** Okinawa Institute of Science and Technology (OIST),

Okinawa, Japan

09/08 - 09/12 **Post-Doctoral Research Associate,** Computational Material Science, University of Twente, the Netherlands
- **Advisor:** Prof. Dr. Geert Brocks

07/02 - 08/02 **Visiting researcher,** National Institute of Standards and Technology (NIST), Gaithersburg, Maryland, U.S.A

Courses Taught

Regular Assignments and Continuing Education:

Spring/21	Solid State Physics II (PHYS-536)
Fall/20	Solid State Physics I (PHYS-535)
Fall/20	Solid State Physics (PHYS-437)
Fall/20	Analytical Mechanics (PHYS-545)
Spring/20	Introduction to Quantum computation (PHYS-492)
Spring/20	Quantum Mechanics II (PHYS-540)
Fall/19	Quantum Mechanics I (PHYS-539)
Fall/19	Special Topics (Material prediction via Machine Learning) (PHYS-550)
Spring/19	University Physics II (PHYS-252)
Spring/19	Special Topics in Physics (PHYS-550)
Spring/18	Quantum Mechanics II (PHYS-540)
Fall/17	Quantum Mechanics I (PHYS-539)
Spring/17	Solid State Physics II (PHYS-536)
Fall/16	Solid State Physics I (PHYS-535)

Previous teaching as a teaching assistant:

2001-2008: Teaching assistant (Department of Physics, Bilkent University, Ankara, Turkey)
- Freshman Physics Lecture and Laboratory
- Quantum Physics
- Quantum Mechanics
- Quantum Mechanics Laboratory
- Electromagnetic theory
- Classical mechanics
- Nanoscience and Nanotechnology
- Statistical Thermodynamics

Professional Associations:

- Member of American Physical Society
- Member of American Chemical Society
- Reviewer for the following journals: Journal of physical chemistry letters, Journal of physical chemistry C, Solid state communications, Journal of Applied Physics, ACS Applied Materials & Interfaces, Advanced Materials, Chemical Communication, Journal of Physics and Chemistry of Solids, Physical Chemistry Chemical Physics, Nanoscale, Applied Physics Letters, Physical Review B, Journal of Materials Chemistry A, Journal of Computational Chemistry, Chemical Physics Letters, Journal of Physics: Condensed Matter, Physical Review Applied, Nano Energy, ACS Applied Energy Materials, ACS Omega, RSC Advances, Molecular Simulation, ACS Nano, Nanoscale Horizons.

Community:

- Visiting Tribal Colleges

Journal Publications

* I am the corresponding author in this publication.

I am the corresponding and the first author in this publication

Total Citations as of 8/18/2021: 2276 (Google Scholar)

2021

1. "Coal-Derived Graphene/MoS_2 Heterostructure Electrodes for Li-ion Batteries: Experiment and Simulation Study", P. R. Ilango, **Deniz Cakir**, X. Zhanga, S. Xua, M. Mann and Xiaodong Hou, Submitted to ACS Applied Materials & Interfaces (2021).

2. "Discovery of novel Nanolaminated Fe_2AB_2 and Mn_2AB_2 (A=Ga, Si, In) materials and their exfoliation into magnetic MBenes", Edirisuriya M. D. Siriwardane, and **Deniz Çakır**, Submitted to J. Phys.: Condens. Matter (2021)*.

3. "Stability of adsorption of Mg and Na on sulfur-functionalized MXenes", G. Chaney, Deniz Çakır, François M. Peeters and C. Ataca, Submitted to PCCP (2021)*.

4. "First-principles discovery of stable two-dimensional materials with giant piezoelectric response", T. Kocabas, **Deniz Çakır**, and C. Sevik, J. Phys.: Condens. Matter 33 115705 (2021)*.

5. "Comprehensive Study of Lithium Adsorption and Diffusion on Janus Mo/WXY (X, Y= S, Se, Te) Using First-Principles and Machine Learning Approaches", G. Chaney, A. Ibrahim, F. Ersan, **Deniz Çakır**, C. Ataca, ACS Applied Materials & Interfaces 13, 36388-36406 (2021).

6. "Engineering magnetic anisotropy and exchange couplings in double transition metal MXenes via surface defects", Edirisuriya M. D. Siriwardane, Pragalv Karki, Yen Lee Loh and **Deniz Çakır**, J. Phys.: Condens. Matter 33 035801 (2021)*.

7. "$CrSi_2$ crystallites on Si(110)", Sameera Pathiranage, Edirisuriya MD Siriwardane, Rasika Mohottige, **Deniz Çakır**, Nuri Oncel, Surface Science 703, 121739 (2021).

2020

8. "Enhanced Electrochemical Storage Properties of Na and Mg Intercalated B-Doped-Graphene Based Heterostructures and Bilayers", Edirisuriya M. D. Siriwardane and **Deniz Çakır**, J. Phys. Chem. C 124, 1260-1268 (2020)*.
9. "Revealing the Formation Energy - Exfoliation Energy - Structure Correlation of MAB Phases using Machine Learning and DFT", Edirisuriya M. D. Siriwardane, Rajendra P. Joshi, Neeraj Kumar and **Deniz Çakır**, ACS Applied Materials & Interfaces 12, 29424-29431 (2020)*.
10. "A systematical ab-initio review of promising 2D MXene monolayers towards Li-ion battery applications", Uğur Yorulmaz, İlker Demiroğlu, **Deniz Çakır**, Oğuz Gülseren, and Cem Sevik, Review paper, J Phys Energy IOP 2, 032006 (2020)*.
11. "Assessment of Sulfur-functionalized MXenes for Li-ion Battery applications", Edirisuriya M. D. Siriwardane, Ilker Demiroglu, Cem Sevik, François M. Peeters, and **Deniz Çakır**, J. Phys. Chem. C 124, 21293-21304 (2020)*.

2019

12. "Temperature-dependent phonon spectrum of transition metal dichalcogenides calculated from the spectral energy density: Lattice thermal conductivity as an application", A. Mobaraki, C. Sevik, H. Yapicioglu, **Deniz Çakır**, O. Gülseren, Physical Review B 100, 035402 (2019).
13. "Tailoring Storage Capacity and Ion Kinetics in Graphene Heterostructures by Functionalization of Graphene", C. Sevik, **Deniz Çakır**, Physical Review Applied 12, 014001 (2019)*.
14. "Strain-Spintronics: Modulating Electronic and Magnetic Properties of $Hf_2MnC_2O_2$ MXene by Uniaxial Strain", Edirisuriya M. D. Siriwardane, Pragalv Karki, Yen Lee Loh and **Deniz Çakır**, J. Phys. Chem. C 123, 1912451 (2019)*.
15. "Silicene-Like Domains on $IrSi_3$ Crystallites", D. Nicholls, Fatima, **Deniz Çakır**, and N. Oncel, The Journal of Physical Chemistry C 123, 7225-7229 (2019).
16. "Strain engineering of electronic and magnetic properties of double-transition metal ferromagnetic semiconductor MXenes", Edirisuriya M. D. Siriwardane, and **Deniz Çakır**, Journal of Applied Physics 125, 082527 (2019)*.
17. "Alkali Metal Intercalation in MXene/Graphene Heterostructures: A New Platform for Ion Battery Applications", I. Demiroglu, F. M. Peeters, O. Gulseren, **Deniz Çakır**, and C Sevik, The journal of physical chemistry letters 10, 727-734 (2019).
18. "Achieving Fast Kinetics and Enhanced Li Storage Capacity for $Ti_3C_2O_2$ by Intercalation of Quinone Molecules", EMD Siriwardane, I. Demiroglu, C. Sevik, **Deniz Çakır**, ACS Applied Energy Materials 2, 1251-1258 (2019)*.

2018

19. "Determination of Dynamically Stable Electrenes towards Ultra-fast Charging Battery Applications", T. Kocabas, A. Ozden, I. Demiroglu, **Deniz Çakır**, C. Sevik, The Journal of Physical Chemistry Letters 9, 4267 (2018).

20. "Electronic and mechanical properties of stiff rhenium carbide monolayers: a first-principles investigation", E. M. D. Siriwardane, P. Karki, C. Sevik and **Deniz Çakır**, Applied Surface Science 458, 762 (2018)*.

21. "In pursuit of barrierless transition metal dichalcogenides lateral heterojunctions", Yierpan Aierken, C. Sevik, O. Gulseren, F. M. Peeters and **Deniz Çakır**, Nanotechnology 29, 295202 (2018)*.

22. "The influence of surface functionalization on thermal transport and thermoelectric properties of MXene monolayers", S. Sarikurt, **Deniz Çakır**, M. Keceli and C. Sevik, Nanoscale 10, 8859 (2018).

23. "A distinct correlation between the vibrational and thermal transport properties of group VA monolayer crystals", T. Kocabas, **Deniz Çakır**, O. Gulseren, F. Ay and N. K. Perkgoz and C. Sevik, Nanoscale 10, 7803 (2018).

24. "Study of Iridium Silicide Monolayers using Density Functional Theory", M. D. Popis, S. V. Popis, N. Oncel, M. R. Hoffmann, and **Deniz Çakır**, Journal of Applied Physics 123, 074301 (2018)*.

25. "MXenes/graphene heterostructures for Li battery applications: a first principles study", Y. Aierken, C. Sevik, O. Gülseren, F. M. Peeters and **Deniz Çakır**, Journal of Materials Chemistry A 6, 2337 (2018)*.

2017

26. "Intercalation of Si between MoS_2 layers", R. van Bremen, Q. Yao, S. Banerjee, **Deniz Çakır**, N. Oncel, and H.J.W. Zandvliet, Beilstein Journal of Nanotechnology 8, 1952 (2017).

27. "Gate induced monolayer behavior in twisted bilayer phosphorene", C. Sevik, John R. Wallbank O. Gulseren, F. M. Peeters, and **Deniz Çakır,** 2D materials 4, 035025 (2017)[*].

28. "Piezoelectricity in two-dimensional materials: lattice dynamics and ab-initio calculations", Karl H. Michel, **Deniz Çakır**, C. Sevik, and F. M. Peeters, Physics Review B 95, 125415 (2017).

2016

29. "On the structural and electronic properties of Ir-silicide nanowires on Si(001) surface", Fatima, I. C. Oguz, **Deniz Çakır**, S. Hossain, R. Mohattige, O. Gulseren, and N. Oncel, J. Appl. Phys. 120, 095303 (2016).

30. "Peculiar piezoelectric properties of two-dimensional materials", C. Sevik, **Deniz Çakır**, O. Gulseren and F. M. Peeters, The Journal of Physical Chemistry C 120, 13948 (2016).

31. "Strain enhancement of acoustic phonon limited mobility in monolayer TiS_3", E. Aierken, **Deniz Çakır** and F. M. Peeters, Physical Chemistry Chemical Physics 18, 14434 (2016)[*].

32. "Mo_2C as a high capacity anode material: a first-principles study", **Deniz Çakır**, C. Sevik, O. Gulseren and F. M. Peeters, Journal Materials Chemistry A 4, 6029 (2016)[#].

2015

33. "Fluorographane: a promising material for bipolar doping of MoS_2", **Deniz Çakır** and F. M. Peeters, Phys. Chem. Chem. Phys. 17, 27636 (2015)[#].

34. "Significant effect of stacking on the electronic and optical properties of few layer black phosphorus", **Deniz Çakır**, Cem Sevik and F. M. Peeters, Physical Review B 92, 165406 (2015)[#].

35. "Promising piezoelectric performance in single layer transition-metal dichalcogenides and dioxides", M. M. Alyoruk, E. Aierken, **Deniz Çakır**, F. M. Peeters, and C. Sevik, J. Phys. Chem. C 119, 23231 (2015).

36. "Thermal properties of black and blue phosphorenes from a first-principles quasi-harmonic approach", E. Aierken, **Deniz Çakır**, C. Sevik, and F. M. Peeters, Phys. Rev. B 92, 081408(R) (2015)[*].

37. "Scanning Tunneling Microscopy and Density Functional Theory Study on Zinc(II)-Phthalocyanine Tetrasulfonic Acid on Bilayer Epitaxial Graphene on Silicon Carbide(0001)", D. Nicholls, R. R. Li, B. Ware, C. Pansegrau, **Deniz Çakır**, M. R. Hoffmann, and N. Oncel, J. Phys. Chem. C 119, 9845 (2015).

38. "Realization of a p-n junction in a single layer boron-phosphide", **Deniz Çakır**, D. Kecik, H. Sahin, E. Durgun, and F. M. Peeters, Phys. Chem. Chem. Phys. 17, 13013 (2015)[#].

39. "Exciton stark shift in few-layer black phosphorus", A. Chaves, T. Low, P. Avouris, **Deniz Çakır**, and F. M. Peeters, Phys. Rev. B 91, 155311 (2015).

2014

40. "Magnetoresistance in multilayer fullerene spin valves: a first-principles study", **Deniz Çakır**, D. Otalvaro and G. Brocks, Phys. Rev. B 90, 245404 (2014).

41. "Tuning of the electronic and optical properties of single layer black phosphorus by strain", **Deniz Çakır**, H. Sahin and F. M. Peeters, Phys. Rev. B 90, 205421 (2014)[#].

42. "Engineering electronic properties of Metal/$MoSe_2$ interfaces using self-assembly monolayers", **Deniz Çakır**, C. Sevik, and F. M. Peeters, J. Mater. Chem. C 2, 9842 (2014)[#].

43. "Doping of rhenium disulfide monolayer: A systematic first principles study", **Deniz Çakır**, H. Sahin, and F. M. Peeters, Phys. Chem. Chem. Phys. 16, 16771 (2014)[#].

44. "Dependence of the electronic and transport properties of metal/$MoSe_2$ interfaces on contact structure", **Deniz Çakır** and F. M. Peeters, Phys. Rev. B 89, 245403 (2014)[#].

45. "Angle-Resolved Synchrotron Photoemission and Density Functional Theory on Iridium Modified Si(111) surface ", N. Oncel, **Deniz Çakır**, J. H. Dil, B. Slomski and G. Landolt, J. Physics: Condensed Matter 26, 285501 (2014).

46. "Mechanical and Thermal properties of h-MX_2 (M=Cr, Mo, W; X=O, S, Se, Te) monolayers: a comparative study", **Deniz Çakır**, F. M. Peeters, and C. Sevik, App. Phys. Lett. 104, 203110 (2014).

47. "Formation and stability of point defects in monolayer rhenium disulfide", S. Horzum, **Deniz Çakır**, S. Tongay, J. Wu, H. Sahin and F. M. Peeters, Phys. Rev. B 89, 155433 (2014)*.

48. "From spin-polarized interfaces to giant magnetoresistance in organic spin valves", **Deniz Çakır**, D. Otalvaro, and G. Brocks, Phys. Rev. B 89, 115407 (2014).

2013

49. "Role of intrinsic molecular dipole in energy level alignment at organic interfaces", L. Lindell, **Deniz Çakır**, G. Brocks, M. Fahlman and S. Braun, Appl. Phys. Lett. 102, 223301 (2013).

50. "Magnetic and electronic properties of Fe atoms at bcc-Fe(001)/C_{60} interfaces for organic spintronics", T. Lan Anh Tran, **Deniz Çakır**, P. K. J. Wong, A. B. Preobrajenski, G. Brocks, W. G. van der Wiel, and M. P. de Jong, ACS Appl. Mater. Interfaces 5, 837 (2013).

2012

51. "Ab-initio study of neutral $(TiO_2)_n$ (n=1-10) clusters and their interaction with H_2O and transition metal atoms", **Deniz Çakır** and O. Gülseren, J. Physics: Condensed Matter 24, 305301 (2012).

52. "Charge equilibration and potentials steps in organic semiconductor multilayers", G. Brocks, **Deniz Çakır**, M. Bokdam, M. P.de Jong and M. Fahlman, Organic Electronics 13, 1793 (2012).

53. "Modeling charge transfer at organic donor-acceptor semiconductor interfaces", **Deniz Çakır**, M. Bokdam, M. P.de Jong, M. Fahlman and G. Brocks, Appl. Phys. Lett. 100, 203302 (2012).

54. "Pt_n (n=1-8) and Pt_2Au_m (m=1-5) clusters on reduced rutile TiO_2 (110) surface", **Deniz Çakır** and O. Gülseren, J. Phys. Chem. C 116, 5735 (2012).

2011

55. "Native defects and the dehydrogenation of $NaBH_4$", **Deniz Çakır**, G. A. de Wijs and G. Brocks, J. Phys. Chem. C 115, 24429 (2011).

56. "Effect of impurities on mechanical and electronic properties of Au, Ag, and Cu monatomic chain nanowires", **Deniz Çakır** and O. Gülseren, Phys. Rev. B 84, 085450 (2011).

57. "Interaction of BrPDI, BrGly, and BrAsp with the Rutile TiO_2 (110) Surface for Photovoltaic and Photocatalytic Applications: A First-Principles Study", **Deniz Çakır**, O. Gülseren, E. Mete and S. Ellialtıoglu, J. Phys. Chem. C 115, 9220 (2011).

58. "Fermi level pinning at electrode-organic semiconductor interfaces", M. Bokdam, **Deniz Çakır** and G. Brocks, Appl. Phys. Lett. 98, 113303 (2011).

2009

59. "Ab-initio study of very thin TiO_x (x=1,2) and (110) rutile nanowires", **Deniz Çakır** and O. Gülseren, Phys. Rev. B 80, 125424 (2009).

60. "Adsorption of BrPDI, BrGly, and BrAsp on anatase TiO_2 (001) surface for the dye sensitized solar cell applications", **Deniz Çakır**, O. Gülseren, E. Mete and S. Ellialtıoglu, Phys. Rev. B 80, 035431 (2009).

2007

61. "Half-metallic silicon nanowires", E. Durgun, **Deniz Çakır**, N. Akman and S. Ciraci, Phys. Rev. Lett. 99, 256806 (2007).

2006

62. "Electronic and mechanical properties of molybdenum selenide type nanowires by plane-wave pseudopotential calculations", **Deniz Çakır**, E. Durgun, O. Gülseren and S. Ciraci, Phys. Rev. B 74, 235433 (2006).

Professional Presentations

1. "Energy storage using MXenes", **invited oral presentation**, 44th International Conference and Exposition on Advanced Ceramics and Composites, January 26-30, 2020, at the Daytona Beach, Florida, USA.

2. "Thermal Transport Properties of Functionalized MXene monolayers", **invited oral presentation**, 42nd International Conference and Exposition on Advanced Ceramics and Composites, January 21-26, 2018, at the Daytona Beach, Florida, USA.

3. "Optical and electronic properties of few-layer black phosphorus: DFT perspective", **invited oral presentation,** North Dakota State University, 10 April 2017, 2016, Fargo/ND USA.

4. "Mo_2C as a high-capacity anode material: a first-principles study", **oral presentation** at the APS MARCH meeting, March 13-17, 2017, New Orleans, LA.

5. "Peculiar Piezoelectric Properties of Two-Dimensional Materials", oral presentation at the Flatlands beyond Graphene 2016, 5-8 July 2016, Bled/Slovenia.

6. "Mo_2C as a high-capacity anode material: a first-principles study", oral presentation at the e-mrs meeting, 2-6 May 2016, Lille/France.

7. "Optical and electronic properties of few-layer black phosphorus: DFT perspective", invited oral presentation, University of North Dakota, 7 April 2016, 2016, Grand Forks/ND USA.

8. "Remarkable effect of stacking on the electronic and optical properties of few layer black phosphorus", oral presentation at Nanotr11, 22-25 June 2015, Middle East Technical University, Ankara/Turkey.

9. "Energy applications from first principles calculations", invited oral presentation, Anadolu University, September 2014, Eskisehir/Turkey.

10. "Dependence of the electronic and transport properties of metal-MoSe2 interfaces on the contact structures", oral presentation at Graphene and related materials 9-11 June 2014, IYTE, Izmir/Turkey.

11. "Doping of rhenium disulfide monolayer: A systematic first principles study", poster presentation at Graphene Week 23-27 June 2014, Gothenburg/Sweden.

12. "Charge transfer at organic donor-acceptor semiconductor interfaces" poster presentation at OIST International Symposium on Organic Electronics, 2012, Okinawa/Japan.

13. "Fermi level pinning at electrode-organic semiconductor interfaces" oral presentation at APS March meeting (2012), Boston/USA.

14. "Charge transfer at organic donor-acceptor semiconductor interfaces" poster presentation at CHAIN meeting, November 28-30 (2011), Maarssen/The Netherlands.

15. "Reaction pathways in the reactive composite $Mg(NH_2)_2$ + LiH" oral presentation at APS March meeting, March 19-25 (2011), Dallas/USA.

16. "Fermi level pinning at electrode-organic semiconductor interfaces" poster presentation at First principles theory and modeling in organic electronics, January 31-February 3 (2011), CECAM, Lausanne/Switzerland.

17. "Reaction pathways in the reactive composite $Mg(NH_2)_2$ + LiH" oral presentation at Scientific meeting on Chemistry related to Physics & Material sciences, February 15-16 (2010), Veldhoven/The Netherlands

18. "Reaction pathways in the reactive composite $Mg(NH_2)_2$ + LiH" oral presentation at 4^{th} Symposium Hydrogen and Energy, January 24-29 (2010), Wildhaus/Switzerland.

19. "Adsorption of BrPDI, BrGly, and BrAsp dye molecules on rutile TiO_2 (110) surface for dye sensitized solar cell applications" oral presentation at NANO-TR 4, Istanbul Technical University, June 9-13 (2008), Istanbul/Turkey.

20. "Electronic and mechanical properties of molybdenum selenide type nanowires", oral presentation at NANO-TR 2, Middle East Technical University, May 3-5 (2006), Ankara/Turkey.

21. "Electronic and mechanical properties of iron disilicides ($FeSi_2$)", poster presentation at Condensed Matter Physics Meeting, Middle East Technical University, November 3 (2006), Ankara/Turkey.

Research Highlights:

- The Editors of the Journal of Applied Physics thought that our work on iridium-silicide monolayer is noteworthy and have chosen it to be promoted as an Editor's Pick.

- My article titled 'The influence of surface functionalization on thermal transport and thermoelectric properties of MXene monolayers' has been specially selected to feature in an Editor's Choice web collection focusing on the use of 2D materials in energy conversion and storage in Journal of Materials Chemistry A.

- My article titled 'Mo_2C as a high-capacity anode material: a first-principles study' has been specially selected to feature in an Editor's Choice web collection focusing on the recent advances in batteries in Journal of Materials Chemistry A.

- Article, "On the structural and electronic properties of Ir-silicide nanowires on Si(001) surface", is published on the cover article of the 1^{th} September 2016 issue of Journal of applied physics