Burak Özdemir

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PROFILE

Date of birth: 1-July-1986

Place of birth: Bandirma/Türkiye

Nationality: Turkish

EDUCATION

Central Michigan University, Mount Pleasant, MI, U.S.A — Ph.D in Science of Advanced Materials, May 2018

Middle East Technical University, Ankara, Turkey — M.Sc. in Physics, 1 August 2013

Middle East Technical University, Ankara, Turkey — B.Sc. in Physics, 13 August 2010

EXPERIENCE

POSTDOC, UNIVERSITY OF MODENA AND REGGIO EMILIA, MODENA, ITALY — 16 MARCH 2024—PRESENT

I am working on binder-electrode interactions in Li-ion battery graphite by using DFT and ab-initio/classical MD calculations.

POSTDOC, NANTES UNIVERSITY, NANTES, FRANCE — 1 SEPTEMBER 2021—28 FEBRUARY 2023

I worked on optical properties of selenium with GW+BSE and also performed noncolinear spin calculations, classical (LAMMPS) and ab-initio molecular dynamics (Quantum-Espresso) calculations and implemented interatomic potential for selenium in LAMMPS. I proposed a mixed helicity structure and explored effects of this on the structural, electronic, magnetic, mechanical, dynamic, and optical properties. I also revealed a possible mechanism for chain to ring transformation shedding light on the structural phase transitions. Here, I worked with Dr. Giorgia Fugallo.

POSTDOC, UNIVERSITY OF OSTRAVA, CZECHIA — 4 DECEMBER 2019—31 DECEMBER 2020

I worked on optical absorption (GW+BSE) and conductivity of two-dimensional defective MXene.

POSTDOC, BILKENT UNIVERSITY, ANKARA, TURKEY — JULY 2018—APRIL 2019

I worked on Janus 2D materials, applications of two-dimensional materials as batteries and thermoelectric converter where I performed ab-initio molecular dynamics as well.

PH.D, CENTRAL MICHIGAN UNIVERSITY, MI, USA — 2014—2018

I worked on battery materials and transparent conductors with Dr. Veronica Barone which was my Ph.D thesis. We showed that lithium in Li-ion batteries can be

replaced with much more earth abundant material potassium. I showed that a nano composite material design is capable of delivering 7 times the capacity of current Li-ion batteries and it works with sodium instead of lithium which is much more abundant on earth than Li. I worked on layered and novel 2D materials and change in optical properties with alkali metal intercalation.

PhD. Thesis: "EXPLORING AND TAILORING THE PROPERTIES OF TWO-DIMENSIONAL MATERIALS" by Burak Ozdemir, (2018)

M.SC., MIDDLE EAST TECHNICAL UNIVERSITY, ANKARA, TURKEY — 2010—2013

I worked on catalytically active material Ceria (CeO2) with DFT+U method and dynamical mean field theory and explored effects of local Hubbard U (Hubbard U applied to surface Ce sites having different U than bulk Ce sites) on CO and Au adsorption on the surface of Ceria. This was my master of science thesis work where I worked with Dr. Hande Toffoli.

MSc. Thesis: "INVESTIGATION OF CATALYTIC PROPERTIES AND ELECTRONIC STRUCTURE OF CORRELATED MATERIAL CeO2 WITH AB-INITIO COMPUTATIONAL METHODS" by Burak Ozdemir, (2013)

B.SC., MIDDLE EAST TECHNICAL UNIVERSITY, ANKARA, TURKEY — 2010

I worked with Prof. Dr. Rasit Turan on CdTe quantum dots and their effect on the photoresponse and external efficiency of Si solar cell as an undergraduate project in my 4th year. This was an experimental work.

SKILLS

Linux, LaTex, Shell scripting, Octave, C#, Fortran, Python, Quantum-Espresso, VASP, Yambo, LAMMPS, Gaussian, CALYPSO, BoltzTrap, ShengBTE, phonopy

LANGUAGES

English (Advanced), French (Elementary), Turkish (Native)

PRESENTATIONS

- Yogun Madde Fiziği Izmir Toplantısı (Condensed Matter Physics Izmir Meeting) Izmir/Turkiye, 2013 - Local Hubbard U and Ceria
- 9th Nanoscience and Nanotechnology Conference (NANOTR-9), Erzurum/Turkiye, 2013, Poster presentation
- APS March Meeting, San Antonio/U.S.A, 2015, Oral Presentation - Structural and Electronic Properties of BC3 with van der Waals density functional theory
- International conference on Advanced Materials and Nanotechnology, 2021, Oral Presentation, Online
- Pacifichem 2021, Invited Speaker - Black Phosphorus solar cell and comparison to silicon from first-principles calculations
- Poster presentation at 25th ETSF workshop on electronic excitations, 13-17 June 2022, Leuven/Belgium

WORKSHOPS

- Quantum Espresso workshop, Penn State University, 16-20 June, 2014
- Online Workshop on Excited State Charge Dynamics in Semiconductors, International Center for Theoretical Physics (ICTP), 28-30 Sep 2020
- Online participation in the school "Ab-initio Many-Body Methods and Simulations with Yambo Code" (ICTP), 4-8 April 2022

- Online participation in the workshop “Workshop on Electrochemical Energy Storage: Theory, Experiments,- and Applications” (ICTP), 5-26 May, 2022

TEACHING

- Quantum physics seminar (problem solving) for physics master students at fall semester 2020 at University of Ostrava

PUBLICATIONS

Google scholar: https://scholar.google.com.tr/citations?user=XjZHhXIAAAAJ&hl=tr

WOS: https://www.webofscience.com/wos/author/record/AAF-4311-2020

1. (First author), ”Structural and electronic properties of crystalline graphite-like BC 3 ”, **Burak Ozdemir**, Veronica Barone, Computational Materials Science, 109, 248-252 (2015)
2. (First author), “Potassium Ion Batteries with Graphitic Materials”, Wei Luo, Jiayu Wan, **Burak Ozdemir**, Wenzhong Bao, Yanan Chen, Jiaqi Dai, Hao Lin, Yue Xu, Feng Gu, Veronica Barone, Liangbing Hu, Nano Letters, 15(11), 7671-7677 (2015)
3. “Hexagonal BC3: A robust electrode material for Li, Na, and K ion batteries”, Rajendra P Joshi, **Burak Ozdemir,** Veronica Barone, Juan E Peralta, The journal of physical chemistry letters, 6(14), 2728-2732 (2015)
4. (First author), “Two-dimensional nitrogen-rich transition metal compounds: The case of TiN 2”, **Burak Ozdemir**, Veronica Barone, Journal of Electron Spectroscopy and Related Phenomena, 219, 29-34, (2017)
5. (First author), “Tunable Broadband Nanocarbon Transparent Conductor by Electrochemical Intercalation”, Jiayu Wan, Yue Xu, **Burak Ozdemir**, Lisha Xu, Andrei B Sushkov, Zhi Yang, Bao Yang, Dennis Drew, Veronica Barone, Liangbing Hu, ACS nano, 11(1), 788-796 (2017)
6. (First author), “Intercalation of alkali metals (Li, Na, and K) in molybdenum dinitride (MoN2) and titanium dinitride (TiN2) from first-principles calculations”, **Burak Ozdemir**, Computational Condensed Matter, 17, e00335, (2018)
7. (First author), “Thickness Dependence of Solar Cell Efficiency in Transition Metal Dichalcogenides MX2 (M: Mo, W; X: S, Se, Te)”, **Burak Ozdemir,** Veronica Barone, Solar Energy Materials and Solar Cells, 212, 110557 (2020)
8. “Oxygeneation of monolayer gallium monochalcogenides: Design of two-dimensional, ternary Ga2XO (X:S. Se. Te) structures” M. Demirtas, **B. Ozdemir**, Y. Mogulkoc, E. Durgun, Phys. Rev. B, 101, 075423 (2020)
9. (First author), “Black Phosphorus and Phosphorene/Graphene Heterostructure as Alkali metal (Li, Na, and K) Ion Battery” **Burak Ozdemir**, arXiv preprint arXiv:2007.10308 (2020)
10. “Single- and Multi-Layer Arsenene as an Anode Material for Li, Na, and K-ion Battery Applications”, Muammer Kanli, Mustafa Kurban, **Burak Ozdemir**, Abudllatif Onen, Engin Durgun, Computational Materials Science, 186, 110000 (2021)
11. “Machine Learning Screening of Metal-Ion Battery Electrode Materials” Isaiah A Moses, Rajendra P Joshi, **Burak Ozdemir**, Neeraj Kumar, Jesse Eickholt, Veronica Barone, ACS Applied Materials & Interfaces, (2021)
12. (First Author), “Comparison of Solar Cell Efficiencies of Black Phosphorus and Silicon at the Nano and Micro Scales from First-Principles Calculations” **Burak Ozdemir**, arXiv preprint arXiv:2407.03733, (2024)
13. (First author), “The Role of Mixed Helicity/Chirality on the Physical Properties of Trigonal Selenium” **Burak Ozdemir**, Giorgia Fugallo, at al. (in the writing stage)