# Daniel Mukasa

#### **Education**

Aug 2019 - July California Institute of Technology, MS/Ph.D Applied Physics and Materials 2024 Science, Advisor: Wei Gao.

- NSF Graduate Research Fellowship
- O Doctoral Thesis: Computational design of biosensors for wearable device applications (full thesis in preparation)

Aug 2015- May

Oberlin College, Bachelors with High Honors in Physics, Math Minor, Advisor: 2019 Stephen FitzGerald.

- John F. Oberlin Merit Scholar
- O Honors Thesis: Development of a Highly Selective Deuterium-Hydrogen Separation Process (full thesis here)

# Work Experience

Aug 2024 - MIT: Postdoctoral Fellow, Mentored by Heather Kulik and Giovanni Present **Traverso**, Machine Learning/Drug Discovery.

Developing a machine learning pipeline for the discovery of mRNA therapeutics.

Aug 2019 - July Caltech: Graduate Research Fellow, Mentored by Wei Gao, MEDICAL 2024 Engineering/Materials Science.

- Using computational chemistry (density functional theory, molecular dynamics, etc.) and machine learning to accelerate the development of diagnostic sensors.
- Developed QuantumDock framework as reported in our Advanced Materials article
- Designed novel biosensors to monitor COVID, diabetes and exhaustion as reported in our Nature Biomedical Engineering article
- Conducting clinical trials to evaluate device efficacy
- discovering new sweat biomarkers for diagnostic application
- Developing medical micro/nanorobots for in vivo application
- Detailed state of the art developments in our Chemical Society Reviews article and in our book chapter in Springer Nature.

Jun 2023 - Aug Merck Data Science Intern, Machine Learning/Cheminformatics.

- 2023 Worked on machine learning algorithms to accelerate the drug discovery pipeline
  - Developed a novel pipeline for the accelerated prediction of binding sites on proteins
  - Worked with medicinal chemists to implement software internally

Aug 2018 - May Honors Research Scholar, Mentored by Stephen Fitzgerlad, PHYSICS.

- 2019 Developed method of separating hydrogen and deuterium gas
  - Designed temperature controlled setup to increase separation selectivity
  - Published article in Journal Of Physical Chemistry C.

June 2018 - UCSB FLAM Computational Intern, Mentored by Susanne Stemmer, Aug 2018 MATERIALS SCIENCE.

> Worked as computational scientist designing models to understand novel physical phenomena in thin film electronic devices. Designed model to maximized device conductivity in thin film systems.

2017 - 2018 Caltech Computational Research Fellow, Mentored by Brent Fultz, MATERIALS SCIENCE.

> Studied low temperature magnetic properties of high entropy alloys using Mössbauer spectroscopy, used scanning electron microscope for material characterization, developed computational models to describe experimental results, summary of this work can be found here.

Machine Learning Researcher, Mentored by Colin Dawson, MACHINE Aug 2017 - Dec 2017 Learning.

> Investigated mathematical and statistical methods used in deep learning neural networks including feed forward, convolutional, and recurrent neural networks, applied neural networks to small projects including image recognition and data classification.

Jul 2016 - Aug 2016, January

Quantum Physics Researcher, Mentored by Stephen FitzGerald, PHYSICS.

- August 2016

2016, July 2016 Worked under Stephen FitzGerald studying Metal Organic Frameworks (MOFs) for hydrogen storage and isotope separation. Developed method of temperature programmed desorption to study isotope separation using MOFs. Utilized infrared spectroscopy to study MOF hydrogen interactions to improve hydrogen storage capabilities.

## Publications

- 1. Daniel Mukasa, Minqiang Wang, Samuel A. Solomon, José Lasalde Ramírez, Wei Gao, "Machine Learning Automated Biosensor Design", in preparation
- 2. Mingiang Wang, Cui Ye, Yiran Yang, **Daniel Mukasa**, Canran Wang, Changhao Xu, Jihong Min, Samuel A. Solomon, Jiaobing Tu, Guofang Shen, Songsong Tang, Tzung K. Hsiai, Zhaoping Li, Jeannine S. McCune, and Wei Gao, "Printable molecule-selective core-shell nanoparticles for wearable and implantable sensing", Submitted to Nature Materials
- 3. Daniel Mukasa, Minqiang Wang, Jihong Min, Yiran Yang, Samuel A. Solomon, Hong Han, Cui Ye, Wei Gao, "A Computationally Assisted Approach for Designing Wearable Biosensors toward Non-invasive Personalized Molecular Analysis", Advanced Materials, **Featured on journal cover**, (full paper)
- 4. Jihong Min, Jiaobing Tu, Changhao Xu, Heather Lukas, Soyoung Shin, Yiran Yang, Samuel A. Solomon, **Daniel Mukasa**, and Wei Gao, "Skin-Interfaced Wearable Sweat Sensors for Precision Medicine", Chemical Reviews, Featured on journal cover, (full paper)
- Minqiang Wang, Yiran Yang, Jihong Min, Yu Song, Jiaobing Tu, Daniel Mukasa, Cui Ye, Changhao Xu, Nicole Heflin, Jeannine S. McCune, Tzung K. Hsiai, Zhaoping Li and Wei Gao, "A wearable electrochemical biosensor for the monitoring of metabolites and nutrients", Nature Biomedical Engineering, Most accessed journal paper in 2022, (full paper)
- 6. Y Song, Mukasa, H Zhang, W Gao, "Self-powered wearable Accounts of Materials Research, ACS Editors Choice, biosensors". Most accessed journal paper in 2021, (full paper)
- 7. Zhiguang Wu, Ye Chen, **Daniel Mukasa**, On Shun Pak and Wei Gao, "Medical micro/nanorobots in complex media", Chemical Society Reviews, (full paper)
- 8. M You, **D Mukasa**, W Gao, "Microrobots in the Gastrointestinal Tract", Springer, Cham, (full book chapter)

9. Stephen A. FitzGerald, **Daniel Mukasa**, Katharine H. Rigdon, Naiyuan Zhang, and Brandon R. Barnett, "Hydrogen Isotope Separation within the Metal-Organic Framework Cu(I)-MFU-4l", Journal of Physical Chemistry C, (full paper)

Summary 1100+ citations; h-index: 6; i10-index: 6; Google Scholar Profile

## Scientific Presentations

- 2024 Invited seminar at UC irvine for the Early Career Distinguished Scholar program
- 2023 AICHE Poster presentation on the computational design of biosensors with wearable application
- 2023 Invited presentation at The Conference for Emerging Black Academics in STEM (CEBAS)
- 2018 Oral presentation at the National Society of Black Physicists meeting on Electron Transport in Thin Film Oxides
- 2018 Oral presentation at the American Physical Society meeting on the magnetic properties of High Entropy Alloys
- 2016 Oral presentation at ABRCMS National Convention on Metal Organic Frameworks
- Oct 2015-2018 Poster and oral presentations at Oberlin's Celebration of Undergraduate Research

## Awards and Honors

- Sept 2024 UC Irvine Early Career Distinguished Scholar Awarded to deliver the annual Early Career Distinguished Scholar seminar. The seminar hosts outstanding postdoctoral scholars and/or Ph.D. students who aspire to pursue academic careers.
- Sept 2023 Materials Today Agents of Change Award Shortlist The only graduate student amongst faculty members highlighted. Nominated for the proposed future funding of the Conference for Emerging Black Academics in STEM (CEBAS). Results to be announced November 30th.
- May 2021 **NSF Graduate Research Fellow** Awarded highly prestigous graduate research fellowship for 3 years of funding in materials science and medical engineering research
- Apr 2021 New Horizons Diversity, Equity and Inclusion Award Awarded for leading Black Scientists and Engineers of Caltech (BSEC) through 2020 as covered in the Nature feature story.
- April 2021 KNI Catalyst Awarded for outstanding leadership in the Caltech community and leading the draft of the 2020 petition to increase on campus diversity.
- May 2019 **Carl E. Howe Prize In Physics** Awarded for outstanding research though the Physics honors program and leadership as president of Oberlin's Black Scientists Guild
- May 2019 **Sigma Xi Scientific Honor Society** Inducted for outstanding undergraduate scientific achievement
- Mar 2018 **APS March Meeting Top Undergraduate Presentation** Awarded for an outstanding presentation at the 2018 American Physical Society March meeting.

- Nov 2016 ABRCMS Outstanding Undergraduate Presentation Certificate of Achievement awarded for an oral presentation given at the Annual Biomedical Research Conference for Minority Students.
- Oberlin 1835 Fund Grant Awarded for proposed independent research project during the winter term of 2018 at Caltech on the magnetic nature of high entropy alloys
- John F. Oberlin Merit Scholarship Scholarship awarded for outstanding June 2015 academic achievement and potential to succeed in college.
- Oberlin College STRONG Scholarship Selected as one of 10 high potential June 2015 researcher from the pool of incoming students. Conducted research in Quantum mechanics and materials science under Stephen FitzGerald.

#### Technical Skills

Laboratory Skills: Scanning Electron Microscopy, X-Ray Diffraction, Hall Effect Measurements, Infrared Spectroscopy, Electrochemestry (Cyclic Voltammetry, Differential Pulse Voltammetry, etc.), UV-VIS Spectroscopy

Machine Learning: Scikit-learn, TensorFlow, PyTorch

General Programming: Python, NumPy, BASH, Super computer management (SLURM)

Computational Chemistry: Avagadro, Orca, OpenBabel, VMD, PySCF, RD-Kit

# Diversity and Inclusion Initiatives

August 2020

May 2020 - Caltech WAVE Mentor, California Institute of Technology, Pasadena, CA.

Mentored three students in Caltech's WAVE fellowship program, gave advice on the graduate school application process, helped find and apply to fellowship opportunities, helped facilitate a healthy work life balance for their summer through programs including zoom hangout rooms, movie nights, and regular meetings.

August 2019 - Black Scientists and Engineers of Caltech, California Institute of Technology, Present Pasadena, CA.

> Helped lead campus wide effort to push for more diversity initiatives at Caltech, conducted comprehensive review of such initiatives at other graduate institutions and reported measures to help increase enrollment, retention, and facilitate the success of traditionally underrepresented students at Caltech as shown in our report. Resulted in increased funding to established diversity programs, guaranteed funding for new programs, creation of fellowships for under represented students, and further commitments as seen in Caltech's response.

2017-June 2018

Black Scientists Guild Co-Chair Revived the Black Scientists Guild after two years of no operation. Responsible for organizing group events, including sending students to conferences to present their research and bringing in diverse speakers to Oberlin, and formulating the general future direction of organization. Worked with community members to increase black participation in sciences amongst younger children via collaboration with Get with the Program Inc. Created a generally supportive community within the college for black scientists to further their careers.

# Teaching and Leadership Experience

August 2021 - President: Black Scientists and Engineers of Caltech, Caltech, Pasadena, August 2022 CA.

Jan 2022 – Mar **Graduate Teaching Assistant: Sensors in Medicine**, Caltech, Pasadena, 2022 CA.

Aug 2017-June **President: Black Scientists Guild**, Oberlin College, Oberlin, OH. 2018

Jan 2017 - May **Teaching Assistant: Energy Science and Technology**, Oberlin College, 2017 Oberlin, OH.

Aug 2016 – Dec **Teaching Assistant: Multivariable Calculus**, Oberlin College, Oberlin, OH. 2016

February 2016 - Math and Physics Tutor, Oberlin College, Oberlin, OH.

May 2016 Tutored math and physics courses ranging from Intermediate Algebra to Calculus II and college level Physics at a nearby high school. This was an unpaid position meant to help students with an underprivileged background do well in school and on nation-wide standardized tests.

Aug 2019 - Mentored students

Now • Daphne Lucana (Currently: PhD at UC Berkeley)

• Maya Watts (Currently: PhD at Northwestern; GEM Fellow)

• Franz O'Meally (Currently: PhD at Caltech; DOE CSGF Fellow | GEM Fellow)

• Chibuike Uwakwe (Currently: MD-PhD at Stanford University)

• Anna Soper (Currently: PhD Stanford; Hertz Fellow)

• Ozioma Ozor-Ilo (Currently: PhD MIT; GEM Fellow)

• Jesse George-Akpenyi (PhD at Harvard-MIT)

• Makyla Boyd (Currently: PhD at UPenn)

#### References

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