

# Amir Barati Farimani

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/3809521/publications.pdf>

Version: 2024-02-01

68  
papers

3,856  
citations

159525

30  
h-index

128225

60  
g-index

72  
all docs

72  
docs citations

72  
times ranked

5014  
citing authors

| #  | ARTICLE                                                                                                                                                                              | IF   | CITATIONS |
|----|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|-----------|
| 1  | Adaptive grey wolf optimizer. <i>Neural Computing and Applications</i> , 2022, 34, 7711-7731.                                                                                        | 3.2  | 40        |
| 2  | VecMetaPy: A vectorized framework for metaheuristic optimization in Python. <i>Advances in Engineering Software</i> , 2022, 166, 103092.                                             | 1.8  | 3         |
| 3  | Molecular contrastive learning of representations via graph neural networks. <i>Nature Machine Intelligence</i> , 2022, 4, 279-287.                                                  | 8.3  | 181       |
| 4  | Graph neural network-accelerated Lagrangian fluid simulation. <i>Computers and Graphics</i> , 2022, 103, 201-211.                                                                    | 1.4  | 26        |
| 5  | Online metaheuristic algorithm selection. <i>Expert Systems With Applications</i> , 2022, 201, 117058.                                                                               | 4.4  | 6         |
| 6  | Activation Pathways of Neurotensin Receptor 1 Elucidated Using Statistical Machine Learning. <i>ACS Chemical Neuroscience</i> , 2022, 13, 1333-1341.                                 | 1.7  | 4         |
| 7  | Forecasting COVID-19 new cases using deep learning methods. <i>Computers in Biology and Medicine</i> , 2022, 144, 105342.                                                            | 3.9  | 61        |
| 8  | Graph neural networks accelerated molecular dynamics. <i>Journal of Chemical Physics</i> , 2022, 156, 144103.                                                                        | 1.2  | 19        |
| 9  | Simultaneous Electrochemical Exfoliation and Covalent Functionalization of MoS <sub>2</sub> Membrane for Ion Sieving. <i>Advanced Materials</i> , 2022, 34, e2201416.                | 11.1 | 45        |
| 10 | MeltpoolNet: Melt pool characteristic prediction in Metal Additive Manufacturing using machine learning. <i>Additive Manufacturing</i> , 2022, 55, 102817.                           | 1.7  | 13        |
| 11 | Prediction of GPCR activity using machine learning. <i>Computational and Structural Biotechnology Journal</i> , 2022, 20, 2564-2573.                                                 | 1.9  | 16        |
| 12 | Improving Molecular Contrastive Learning via Faulty Negative Mitigation and Decomposed Fragment Contrast. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 2713-2725. | 2.5  | 26        |
| 13 | Dominant motion identification of multi-particle system using deep learning from video. <i>Neural Computing and Applications</i> , 2022, 34, 18183-18193.                            | 3.2  | 4         |
| 14 | Reduced thermal conductivity of supported and encased monolayer and bilayer MoS <sub>2</sub> . <i>2D Materials</i> , 2021, 8, 011001.                                                | 2.0  | 29        |
| 15 | StressGAN: A Generative Deep Learning Model for Two-Dimensional Stress Distribution Prediction. <i>Journal of Applied Mechanics, Transactions ASME</i> , 2021, 88, .                 | 1.1  | 47        |
| 16 | Potential neutralizing antibodies discovered for novel corona virus using machine learning. <i>Scientific Reports</i> , 2021, 11, 5261.                                              | 1.6  | 62        |
| 17 | DNA Detection with Single-Layer Ti <sub>3</sub> C <sub>2</sub> MXene Nanopore. <i>ACS Nano</i> , 2021, 15, 4861-4869.                                                                | 7.3  | 35        |
| 18 | Deep learning of material transport in complex neurite networks. <i>Scientific Reports</i> , 2021, 11, 11280.                                                                        | 1.6  | 7         |

| #  | ARTICLE                                                                                                                                                                                             | IF  | CITATIONS |
|----|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|-----------|
| 19 | Titanium Carbide MXene for Water Desalination: A Molecular Dynamics Study. ACS Applied Nano Materials, 2021, 4, 6145-6151.                                                                          | 2.4 | 44        |
| 20 | Efficient water desalination with graphene nanopores obtained using artificial intelligence. Npj 2D Materials and Applications, 2021, 5, .                                                          | 3.9 | 36        |
| 21 | Deep reinforcement learning for predicting kinetic pathways to surface reconstruction in a ternary alloy. Machine Learning: Science and Technology, 2021, 2, 045018.                                | 2.4 | 14        |
| 22 | Data-driven identification of 2D Partial Differential Equations using extracted physical features. Computer Methods in Applied Mechanics and Engineering, 2021, 381, 113831.                        | 3.4 | 8         |
| 23 | Graph convolutional networks applied to unstructured flow field data. Machine Learning: Science and Technology, 2021, 2, 045020.                                                                    | 2.4 | 21        |
| 24 | Isolating Specific vs. Non-Specific Binding Responses in Conducting Polymer Biosensors for Bio-Fingerprinting. Sensors, 2021, 21, 6335.                                                             | 2.1 | 2         |
| 25 | Ozark Graphene Nanopore for Efficient Water Desalination. Journal of Physical Chemistry B, 2021, 125, 11256-11263.                                                                                  | 1.2 | 26        |
| 26 | Deep learning for reduced order modelling and efficient temporal evolution of fluid simulations. Physics of Fluids, 2021, 33, .                                                                     | 1.6 | 52        |
| 27 | Understanding mutation hotspots for the SARS-CoV-2 spike protein using Shannon Entropy and K-means clustering. Computers in Biology and Medicine, 2021, 138, 104915.                                | 3.9 | 31        |
| 28 | Heteroatom-Doped Transition Metal Nitrides for CO Electrochemical Reduction: A Density Functional Theory Screening Study. Journal of Physical Chemistry C, 2020, 124, 26344-26351.                  | 1.5 | 8         |
| 29 | Why is Single-Layer MoS <sub>2</sub> a More Energy Efficient Membrane for Water Desalination?. ACS Energy Letters, 2020, 5, 2217-2222.                                                              | 8.8 | 78        |
| 30 | A Review on Challenges and Successes in Atomic-Scale Design of Catalysts for Electrochemical Synthesis of Hydrogen Peroxide. ACS Catalysis, 2020, 10, 7495-7511.                                    | 5.5 | 254       |
| 31 | Machine Learning Force Fields and Coarse-Grained Variables in Molecular Dynamics: Application to Materials and Biological Systems. Journal of Chemical Theory and Computation, 2020, 16, 4757-4775. | 2.3 | 120       |
| 32 | Reaction diffusion system prediction based on convolutional neural network. Scientific Reports, 2020, 10, 3894.                                                                                     | 1.6 | 34        |
| 33 | Orbital graph convolutional neural network for material property prediction. Physical Review Materials, 2020, 4, .                                                                                  | 0.9 | 64        |
| 34 | Thermal boundary conductance of two-dimensional MoS <sub>2</sub> interfaces. Journal of Applied Physics, 2019, 126, .                                                                               | 1.1 | 32        |
| 35 | Bio-inspired Stochastic Growth and Initialization for Artificial Neural Networks. Lecture Notes in Computer Science, 2019, , 88-100.                                                                | 1.0 | 0         |
| 36 | Water Desalination with Two-Dimensional Metal-Organic Framework Membranes. Nano Letters, 2019, 19, 8638-8643.                                                                                       | 4.5 | 119       |

| #  | ARTICLE                                                                                                                                                                                                                                               | IF   | CITATIONS |
|----|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|-----------|
| 37 | Thermal transport in $\text{MoS}_2$ from molecular dynamics using different empirical potentials. <i>Physical Review B</i> , 2019, 99, .                                                                                                              |      |           |
| 38 | Machine Learning Based Approaches to Accelerate Energy Materials Discovery and Optimization. <i>ACS Energy Letters</i> , 2019, 4, 187-191.                                                                                                            | 8.8  | 24        |
| 39 | Binding Pathway of Opiates to $\mu$ -Opioid Receptors Revealed by Machine Learning. <i>Biophysical Journal</i> , 2018, 114, 62a-63a.                                                                                                                  | 0.2  | 9         |
| 40 | Identification of amino acids with sensitive nanoporous $\text{MoS}_2$ : towards machine learning-based prediction. <i>Npj 2D Materials and Applications</i> , 2018, 2, .                                                                             | 3.9  | 47        |
| 41 | Energy Dissipation in Monolayer $\text{MoS}_2$ Electronics. <i>Nano Letters</i> , 2017, 17, 3429-3433.                                                                                                                                                | 4.5  | 177       |
| 42 | Antibody Subclass Detection Using Graphene Nanopores. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1670-1676.                                                                                                                              | 2.1  | 25        |
| 43 | DNA Origami-Graphene Hybrid Nanopore for DNA Detection. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 92-100.                                                                                                                              | 4.0  | 88        |
| 44 | Solution-Phase Conformation and Dynamics of Conjugated Isoindigo-Based Donor-Acceptor Polymer Single Chains. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5479-5486.                                                                       | 2.1  | 24        |
| 45 | Dissolution of Monocrystalline Silicon Nanomembranes and Their Use as Encapsulation Layers and Electrical Interfaces in Water-Soluble Electronics. <i>ACS Nano</i> , 2017, 11, 12562-12572.                                                           | 7.3  | 82        |
| 46 | Thermal boundary conductance of the $\text{MoS}_2$ - $\text{SiO}_2$ interface. , 2017, , .                                                                                                                                                            |      | 2         |
| 47 | Nano-electro-mechanical pump: Giant pumping of water in carbon nanotubes. <i>Scientific Reports</i> , 2016, 6, 26211.                                                                                                                                 | 1.6  | 17        |
| 48 | Existence of Multiple Phases of Water at Nanotube Interfaces. <i>Journal of Physical Chemistry C</i> , 2016, 120, 23763-23771.                                                                                                                        | 1.5  | 49        |
| 49 | Ultrathin, transferred layers of thermally grown silicon dioxide as biofluid barriers for biointegrated flexible electronic systems. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 11682-11687. | 3.3  | 175       |
| 50 | Computational Approach to Designing Antibody for Ebola Virus. <i>Biophysical Journal</i> , 2016, 110, 537a.                                                                                                                                           | 0.2  | 3         |
| 51 | Mechanically modulated electronic properties of water-filled fullerenes. <i>MRS Communications</i> , 2015, 5, 305-310.                                                                                                                                | 0.8  | 8         |
| 52 | Silicon Nanomembranes: Mechanisms for Hydrolysis of Silicon Nanomembranes as Used in Bioresorbable Electronics ( <i>Adv. Mater.</i> 11/2015). <i>Advanced Materials</i> , 2015, 27, 1856-1856.                                                        | 11.1 | 3         |
| 53 | Multiscale modeling of droplet interface bilayer membrane networks. <i>Biomicrofluidics</i> , 2015, 9, 064101.                                                                                                                                        | 1.2  | 13        |
| 54 | Functionality of MscL in Droplet Interface Bilayer. <i>Biophysical Journal</i> , 2015, 108, 373a.                                                                                                                                                     | 0.2  | 0         |

| #  | ARTICLE                                                                                                                                                                                | IF   | CITATIONS |
|----|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|-----------|
| 55 | Adsorption Kinetics Dictate Monolayer Self-Assembly for Both Lipid-In and Lipid-Out Approaches to Droplet Interface Bilayer Formation. <i>Langmuir</i> , 2015, 31, 12883-12893.        | 1.6  | 58        |
| 56 | Electromechanical Signatures for DNA Sequencing through a Mechanosensitive Nanopore. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 650-657.                                  | 2.1  | 19        |
| 57 | Mechanisms for Hydrolysis of Silicon Nanomembranes as Used in Bioresorbable Electronics. <i>Advanced Materials</i> , 2015, 27, 1857-1864.                                              | 11.1 | 98        |
| 58 | Water desalination with a single-layer MoS <sub>2</sub> nanopore. <i>Nature Communications</i> , 2015, 6, 8616.                                                                        | 5.8  | 604       |
| 59 | Thermodynamic insight into spontaneous hydration and rapid water permeation in aquaporins. <i>Applied Physics Letters</i> , 2014, 105, 083702.                                         | 1.5  | 27        |
| 60 | Thermodynamics of Water Entry in Aquaporins. <i>Biophysical Journal</i> , 2014, 106, 559a.                                                                                             | 0.2  | 0         |
| 61 | DNA Base Detection Using a Single-Layer MoS <sub>2</sub> . <i>ACS Nano</i> , 2014, 8, 7914-7922.                                                                                       | 7.3  | 305       |
| 62 | Rotational motion of a single water molecule in a buckyball. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 17993.                                                             | 1.3  | 56        |
| 63 | The Role of External Defects in Chemical Sensing of Graphene Field-Effect Transistors. <i>Nano Letters</i> , 2013, 13, 1962-1968.                                                      | 4.5  | 125       |
| 64 | Mechanical behavior of water filled C60. <i>Applied Physics Letters</i> , 2013, 103, .                                                                                                 | 1.5  | 8         |
| 65 | Spatial Diffusion of Water in Carbon Nanotubes: From Fickian to Ballistic Motion. <i>Journal of Physical Chemistry B</i> , 2011, 115, 12145-12149.                                     | 1.2  | 153       |
| 66 | Computational modeling of the wind erosion on a sinusoidal pile using a moving boundary method. <i>Geomorphology</i> , 2011, 130, 299-311.                                             | 1.1  | 13        |
| 67 | Numerical and experimental analysis of wind erosion on a sinusoidal pile. <i>Environmental Fluid Mechanics</i> , 2011, 11, 167-181.                                                    | 0.7  | 9         |
| 68 | A study on the measurement of mean velocity and its convergence in molecular dynamics simulations. <i>International Journal for Numerical Methods in Fluids</i> , 2011, 67, 2130-2140. | 0.9  | 9         |