

# Mehdi Neek-Amal

## List of Publications by Year in descending order

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Version: 2024-02-01

105  
papers

3,462  
citations

109321

35  
h-index

155660

55  
g-index

107  
all docs

107  
docs citations

107  
times ranked

4307  
citing authors

| #  | ARTICLE   | IF   | CITATIONS |
|----|---|------|-----------|
| 1  | Catalytic properties of cyclo-carbon clusters: An investigation on $\sigma$ activation and CO oxidation. Surface Science, 2022, 720, 122050.  | 1.9  | 6         |
| 2  | Indentation of graphene nano-bubbles. Nanoscale, 2022, , .  | 5.6  | 2         |
| 3  | Trilayer Metal-Organic Frameworks as Multifunctional Electrocatalysts for Energy Conversion and Storage Applications. Journal of the American Chemical Society, 2022, 144, 3411-3428.                     | 13.7 | 142       |
| 4  | Comment on "Two-dimensional carbon nitride C <sub>6</sub> N nanosheet with egg-comb-like structure and electronic properties of a semimetal [Nanotechnology 2021, 32, 215702]". Nanotechnology, 2022, , . | 2.6  | 0         |
| 5  | Electronic Properties of Oxidized Graphene: Effects of Strain and an Electric Field on Flat Bands and the Energy Gap. Journal of Physical Chemistry Letters, 2022, 13, 66-74.                             | 4.6  | 5         |
| 6  | Comment on "A novel two-dimensional boron-carbon-nitride (BCN) monolayer: A first-principles insight". Appl. Phys. 130, 114301 (2021)]. Journal of Applied Physics, 2022, 131, 216101.                    | 2.5  | 0         |
| 7  | Hydration effects and negative dielectric constant of nano-confined water between cation intercalated MXenes. Nanoscale, 2021, 13, 922-929.   | 5.6  | 7         |
| 8  | Abnormal Dielectric Constant of Nanoconfined Water between Graphene Layers in the Presence of Salt. Journal of Physical Chemistry B, 2021, 125, 1604-1610.  | 2.6  | 19        |
| 9  | Abnormal in-plane permittivity and ferroelectricity of confined water: From sub-nanometer channels to bulk. Journal of Chemical Physics, 2021, 154, 114503.   | 3.0  | 14        |
| 10 | Oscillation in the electrical conductivity of a thick graphene oxide membrane. Journal of Applied Physics, 2021, 129, 235105.   | 2.5  | 1         |
| 11 | Tunable natural terahertz and mid-infrared hyperbolic plasmons in carbon phosphide. Carbon, 2021, 178, 625-631.   | 10.3 | 12        |
| 12 | The inhibition performance of quinoa seed on corrosion behavior of carbon steel in the HCl solution; theoretical and experimental evaluations. Journal of Molecular Liquids, 2021, 335, 116183.           | 4.9  | 26        |
| 13 | Breakdown of Universal Scaling for Nanometer-Sized Bubbles in Graphene. Nano Letters, 2021, 21, 8103-8110.  | 9.1  | 23        |
| 14 | The interaction between atomic-scale pores and particles. Journal of Physics Condensed Matter, 2021, 34, .  | 1.8  | 0         |
| 15 | Evaluating gas permeance through graphene nanopores and porous 2D-membranes: A generalized approach. Carbon Trends, 2021, 5, 100086.  | 3.0  | 2         |
| 16 | Gas Permeability and Selectivity of a Porous WS <sub>2</sub> Monolayer. Journal of Physical Chemistry C, 2021, 125, 25055-25066.  | 3.1  | 11        |
| 17 | Out-of-plane permittivity of confined water. Physical Review E, 2020, 102, 022803.  | 2.1  | 35        |
| 18 | Gas flow through atomic-scale apertures. Science Advances, 2020, 6, .   | 10.3 | 22        |

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|----|---|------|-----------|
| 19 | Optoelectronic properties of confined water in angstrom-scale slits. <i>Physical Review B</i> , 2020, 102, .  | 3.2  | 6         |
| 20 | Electronic, dielectric, and optical properties of two-dimensional and bulk ice: A multiscale simulation study. <i>Physical Review B</i> , 2020, 101, .                            | 3.2  | 13        |
| 21 | Tuning the electronic properties of grapheneâ€“graphitic carbon nitride heterostructures and heterojunctions by using an electric field. <i>Physical Review B</i> , 2020, 101, .  | 3.2  | 54        |
| 22 | Two-dimensional graphitic carbon nitrides: Strain-tunable ferromagnetic ordering. <i>Physical Review B</i> , 2020, 101, .   | 3.2  | 37        |
| 23 | Mechanical properties of twin graphene subjected to uniaxial stress by molecular dynamic simulation. <i>Materials Research Express</i> , 2019, 6, 105611.                         | 1.6  | 10        |
| 24 | Self-Limiting Growth of Two-Dimensional Palladium between Graphene Oxide Layers. <i>Nano Letters</i> , 2019, 19, 4678-4683.   | 9.1  | 18        |
| 25 | Ionized water confined in graphene nanochannels. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9285-9295.  | 2.8  | 10        |
| 26 | Electric-field-induced emergent electrical connectivity in graphene oxide. <i>Physical Review B</i> , 2019, 99, .   | 3.2  | 3         |
| 27 | Electrostrictive behavior of confined water subjected to GPa pressure. <i>Physical Review B</i> , 2018, 97, .   | 3.2  | 8         |
| 28 | Transport of hydrogen isotopes through interlayer spacing in van der Waals crystals. <i>Nature Nanotechnology</i> , 2018, 13, 468-472.  | 31.5 | 45        |
| 29 | Electrically controlled water permeation through graphene oxide membranes. <i>Nature</i> , 2018, 559, 236-240.  | 27.8 | 263       |
| 30 | Fast water flow through graphene nanocapillaries: A continuum model approach involving the microscopic structure of confined water. <i>Applied Physics Letters</i> , 2018, 113, . | 3.3  | 34        |
| 31 | Slippage dynamics of confined water in graphene oxide capillaries. <i>Physical Review Materials</i> , 2018, 2, .  | 2.4  | 8         |
| 32 | Thermal activated rotation of graphene flake on graphene. <i>2D Materials</i> , 2017, 4, 025015.  | 4.4  | 21        |
| 33 | Electro- and opto-mutable properties of MgO nanoclusters adsorbed on mono- and double-layer graphene. <i>Nanoscale</i> , 2017, 9, 4205-4218.                                      | 5.6  | 24        |
| 34 | Reversible structural transition in nanoconfined ice. <i>Physical Review B</i> , 2017, 95, .  | 3.2  | 28        |
| 35 | Dependence of the shape of graphene nanobubbles on trapped substance. <i>Nature Communications</i> , 2017, 8, 15844.  | 12.8 | 65        |
| 36 | Temperature distribution in graphene doped with nitrogen and graphene with grain boundary. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 74, 100-104.                | 2.4  | 14        |

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|----|---|------|-----------|
| 37 | Large CO <sub>2</sub> uptake on a monolayer of CaO. Journal of Materials Chemistry A, 2017, 5, 2110-2114.   | 10.3 | 7         |
| 38 | Unconventional two-dimensional vibrations of a decorated carbon nanotube under electric field: linking actuation to advanced sensing ability. Scientific Reports, 2017, 7, 13481.       | 3.3  | 1         |
| 39 | The formation of Cr <sub>2</sub> O <sub>3</sub> nanoclusters over graphene sheet and carbon nanotubes. Chemical Physics Letters, 2017, 687, 188-193.                                    | 2.6  | 5         |
| 40 | Spatial design and control of graphene flake motion. Physical Review B, 2017, 96, .   | 3.2  | 4         |
| 41 | Monolayer alkali and transition-metal monoxides: MgO, CaO, MnO, and NiO. Physical Review B, 2017, 95, .   | 3.2  | 25        |
| 42 | Anomalous Dynamical Behavior of Freestanding Graphene Membranes. Physical Review Letters, 2016, 117, 126801.  | 7.8  | 59        |
| 43 | Electric-field-induced structural changes in water confined between two graphene layers. Physical Review B, 2016, 94, .   | 3.2  | 36        |
| 44 | N-doped graphene: Polarization effects and structural properties. Physical Review B, 2016, 93, .  | 3.2  | 16        |
| 45 | Static flexural modes and piezoelectricity in 2D and layered crystals. Physica Status Solidi (B): Basic Research, 2016, 253, 2311-2315.   | 1.5  | 5         |
| 46 | Van der Waals pressure and its effect on trapped interlayer molecules. Nature Communications, 2016, 7, 12168.   | 12.8 | 137       |
| 47 | Commensurability Effects in Viscosity of Nanoconfined Water. ACS Nano, 2016, 10, 3685-3692.   | 14.6 | 198       |
| 48 | Graphene-silicene bilayer: A nanocapacitor with permanent dipole and piezoelectricity effect. Physical Review B, 2015, 92, .  | 3.2  | 20        |
| 49 | Partially hydrogenated and fluorinated graphene: Structure, roughness, and negative thermal expansion. Physical Review B, 2015, 92, .   | 3.2  | 6         |
| 50 | AA-stacked bilayer square ice between graphene layers. Physical Review B, 2015, 92, .   | 3.2  | 48        |
| 51 | Rippling, buckling, and melting of single- and multilayer $\text{MoS}_2$ . Physical Review B, 2015, 91, .   | 3.2  | 41        |
| 52 | Diffusion of fluorine on and between graphene layers. Physical Review B, 2015, 91, .  | 3.2  | 17        |
| 53 | Graphene ripples as a realization of a two-dimensional Ising model: A scanning tunneling microscope study. Physical Review B, 2015, 91, .   | 3.2  | 22        |
| 54 | Molecular dynamics simulation of temperature profile in partially hydrogenated graphene and graphene with grain boundary. Journal of Molecular Graphics and Modelling, 2015, 62, 38-42. | 2.4  | 5         |

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|----|---|------|-----------|
| 55 | Membrane amplitude and triaxial stress in twisted bilayer graphene deciphered using first-principles directed elasticity theory and scanning tunneling microscopy. <i>Physical Review B</i> , 2014, 90, . | 3.2  | 11        |
| 56 | Graphene on hexagonal lattice substrate: Stress and pseudo-magnetic field. <i>Applied Physics Letters</i> , 2014, 104, .  | 3.3  | 20        |
| 57 | The effects of temperature and vacancies on dynamics of crack in graphene sheet. <i>AIP Advances</i> , 2014, 4, .   | 1.3  | 14        |
| 58 | Unusual ultra-low-frequency fluctuations in freestanding graphene. <i>Nature Communications</i> , 2014, 5, 3720.  | 12.8 | 69        |
| 59 | Stabilized silicene within bilayer graphene: A proposal based on molecular dynamics and density-functional tight-binding calculations. <i>Physical Review B</i> , 2014, 89, .                             | 3.2  | 51        |
| 60 | Electronic properties of graphene nano-flakes: Energy gap, permanent dipole, termination effect, and Raman spectroscopy. <i>Journal of Chemical Physics</i> , 2014, 140, 074304.                          | 3.0  | 35        |
| 61 | The different adsorption mechanism of methane molecule onto a boron nitride and a graphene flakes. <i>Journal of Applied Physics</i> , 2014, 116, .   | 2.5  | 16        |
| 62 | Multilayer graphene, Moiré patterns, grain boundaries and defects identified by scanning tunneling microscopy on the m-plane, non-polar surface of SiC. <i>Carbon</i> , 2014, 80, 75-81.                  | 10.3 | 16        |
| 63 | Graphene on boron-nitride: Moiré pattern in the van der Waals energy. <i>Applied Physics Letters</i> , 2014, 104, .   | 3.3  | 66        |
| 64 | Thermal mirror buckling in freestanding graphene locally controlled by scanning tunnelling microscopy. <i>Nature Communications</i> , 2014, 5, 4962.  | 12.8 | 43        |
| 65 | Melting of Partially Fluorinated Graphene: From Detachment of Fluorine Atoms to Large Defects and Random Coils. <i>Journal of Physical Chemistry C</i> , 2014, 118, 4460-4464.                            | 3.1  | 17        |
| 66 | Self-Organized Platinum Nanoparticles on Freestanding Graphene. <i>ACS Nano</i> , 2014, 8, 2697-2703.   | 14.6 | 39        |
| 67 | Electronic structure of a hexagonal graphene flake subjected to triaxial stress. <i>Physical Review B</i> , 2013, 88, .   | 3.2  | 52        |
| 68 | Realization of free-standing silicene using bilayer graphene. <i>Applied Physics Letters</i> , 2013, 103, .   | 3.3  | 80        |
| 69 | Doping effect on the adsorption of NH <sub>3</sub> molecule onto graphene quantum dot: From the physisorption to the chemisorption. <i>Journal of Applied Physics</i> , 2013, 114, .                      | 2.5  | 18        |
| 70 | Spiral graphone and one-sided fluorographene nanoribbons. <i>Physical Review B</i> , 2013, 87, .  | 3.2  | 17        |
| 71 | Melting of graphene clusters. <i>Physical Review B</i> , 2013, 87, .  | 3.2  | 30        |
| 72 | Thermal properties of fluorinated graphene. <i>Physical Review B</i> , 2013, 87, .  | 3.2  | 91        |

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|----|--|-----|-----------|
| 73 | Boron Nitride Monolayer: A Strain-Tunable Nanosensor. Journal of Physical Chemistry C, 2013, 117, 13261-13267.                                 | 3.1 | 45        |
| 74 | Thermomechanical properties of a single hexagonal boron nitride sheet. Physical Review B, 2013, 87, .  | 3.2 | 87        |
| 75 | Induced polarization and electronic properties of carbon-doped boron nitride nanoribbons. Physical Review B, 2012, 86, .                       | 3.2 | 43        |
| 76 | Methane molecule over the defected and rippled graphene sheet. Solid State Communications, 2012, 152, 1493-1496.                               | 1.9 | 17        |
| 77 | Effect of grain boundary on the buckling of graphene nanoribbons. Applied Physics Letters, 2012, 100, .  | 3.3 | 18        |
| 78 | Thermomechanical properties of graphene: valence force field model approach. Journal of Physics Condensed Matter, 2012, 24, 175303.            | 1.8 | 24        |
| 79 | Strain-engineered graphene through a nanostructured substrate. I. Deformations. Physical Review B, 2012, 85, .                                 | 3.2 | 57        |
| 80 | Strain-engineered graphene through a nanostructured substrate. II. Pseudomagnetic fields. Physical Review B, 2012, 85, .                       | 3.2 | 30        |
| 81 | Thermal rippling behavior of graphane. Physical Review B, 2012, 86, .  | 3.2 | 47        |
| 82 | Nanoengineered nonuniform strain in graphene using nanopillars. Physical Review B, 2012, 86, .   | 3.2 | 55        |
| 83 | Van der Waals energy surface of a carbon nanotube sheet. Solid State Communications, 2012, 152, 225-230.                                       | 1.9 | 4         |
| 84 | Directed motion of $C$ on a graphene sheet subjected to a temperature gradient. Physical Review E, 2011, 83, 042601.                           | 2.1 | 47        |
| 85 | Lattice thermal properties of graphane: Thermal contraction, roughness, and heat capacity. Physical Review B, 2011, 83, .                      | 3.2 | 47        |
| 86 | Comment on "Irreversibility in Response to Forces Acting on Graphene Sheets". Physical Review Letters, 2011, 106, 209701; author reply 209702. | 7.8 | 3         |
| 87 | Buckled circular monolayer graphene: a graphene nano-bowl. Journal of Physics Condensed Matter, 2011, 23, 045002.                              | 1.8 | 24        |
| 88 | Nanoindentation of a circular sheet of bilayer graphene. Physical Review B, 2010, 81, .  | 3.2 | 118       |
| 89 | Stochastic motion of noble gases on a graphene sheet. Computational Materials Science, 2010, 49, 839-844.                                      | 3.0 | 10        |
| 90 | Diffusive motion of $C$ on a graphene sheet. Physical Review E, 2010, 82, 051605.  | 2.1 | 44        |

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|-----|--|-----|-----------|
| 91  | Graphene nanoribbons subjected to axial stress. <i>Physical Review B</i> , 2010, 82, .   | 3.2 | 92        |
| 92  | Defected graphene nanoribbons under axial compression. <i>Applied Physics Letters</i> , 2010, 97, .  | 3.3 | 50        |
| 93  | Linear reduction of stiffness and vibration frequencies in defected circular monolayer graphene. <i>Physical Review B</i> , 2010, 81, .  | 3.2 | 43        |
| 94  | Electric field effects on Nano-Scale bio-membrane of spherical cells. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2009, 388, 120-128.                             | 2.6 | 4         |
| 95  | The formation of atomic nanoclusters on graphene sheets. <i>Nanotechnology</i> , 2009, 20, 135602.   | 2.6 | 89        |
| 96  | Ground state study of simple atoms within a nanoscale box. <i>Solid State Communications</i> , 2008, 145, 594-599.   | 1.9 | 4         |
| 97  | Effective potential of longitudinal interactions between microtubule protofilaments. <i>Physical Review E</i> , 2008, 78, 011912.  | 2.1 | 0         |
| 98  | Study of Hydrogen Molecule and Hydrogen Molecular Ion Confined in C <sub>60</sub> Fullerene. <i>Journal of Computational and Theoretical Nanoscience</i> , 2008, 5, 366-374.         | 0.4 | 2         |
| 99  | Enhanced roughness of lipid membranes caused by external electric fields. <i>Computational Materials Science</i> , 2007, 41, 202-207.  | 3.0 | 2         |
| 100 | Ground-state properties of a confined simple atom by C <sub>60</sub> fullerene. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2007, 40, 1509-1521.            | 1.5 | 19        |
| 101 | Asymmetric simple exclusion process describing conflicting traffic flows. <i>Europhysics Letters</i> , 2007, 80, 60002.  | 2.0 | 41        |
| 102 | Roughness of undoped graphene and its short-range induced gauge field. <i>Physical Review B</i> , 2007, 76, .  | 3.2 | 61        |
| 103 | Monte Carlo simulation of size effects on thermal conductivity in a two-dimensional Ising system. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2006, 371, 424-432. | 2.6 | 8         |
| 104 | Molecular Dynamics Simulation of the Thermal Conductivity of Fcc Metallic Nanocrystals. <i>Journal of Computational and Theoretical Nanoscience</i> , 2005, 2, 438-442.              | 0.4 | 0         |
| 105 | Editorial: Nanoconfined Fluids in Energy Applications. <i>Frontiers in Energy Research</i> , 0, 10, .  | 2.3 | 0         |