# Mehdi Neek-Amal

### List of Publications by Citations

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| #   | Paper   | IF              | Citations      |
|-----|---|-----------------|----------------|
| 101 | Electrically controlled water permeation through graphene oxide membranes. <i>Nature</i> , <b>2018</b> , 559, 236-2                     | 2 <b>45</b> 0.4 | 177            |
| 100 | Commensurability Effects in Viscosity of Nanoconfined Water. ACS Nano, 2016, 10, 3685-92  | 16.7            | 141            |
| 99  | Nanoindentation of a circular sheet of bilayer graphene. <i>Physical Review B</i> , <b>2010</b> , 81,                                   | 3.3             | 105            |
| 98  | Van der Waals pressure and its effect on trapped interlayer molecules. <i>Nature Communications</i> , <b>2016</b> , 7, 12168            | 17.4            | 91             |
| 97  | Graphene nanoribbons subjected to axial stress. <i>Physical Review B</i> , <b>2010</b> , 82,  | 3.3             | 84             |
| 96  | The formation of atomic nanoclusters on graphene sheets. <i>Nanotechnology</i> , <b>2009</b> , 20, 135602                               | 3.4             | 79             |
| 95  | Realization of free-standing silicene using bilayer graphene. <i>Applied Physics Letters</i> , <b>2013</b> , 103, 261904                | 3.4             | 75             |
| 94  | Thermal properties of fluorinated graphene. <i>Physical Review B</i> , <b>2013</b> , 87,  | 3.3             | 75             |
| 93  | Thermomechanical properties of a single hexagonal boron nitride sheet. <i>Physical Review B</i> , <b>2013</b> , 87,                     | 3.3             | 7 <del>2</del> |
| 92  | Graphene on boron-nitride: Moir[pattern in the van der Waals energy. <i>Applied Physics Letters</i> , <b>2014</b> , 104, 041909         | 3.4             | 60             |
| 91  | Roughness of undoped graphene and its short-range induced gauge field. <i>Physical Review B</i> , <b>2007</b> , 76,                     | 3.3             | 55             |
| 90  | Strain-engineered graphene through a nanostructured substrate. I. Deformations. <i>Physical Review B</i> , <b>2012</b> , 85,            | 3.3             | 54             |
| 89  | Unusual ultra-low-frequency fluctuations in freestanding graphene. <i>Nature Communications</i> , <b>2014</b> , 5, 3720                 | 17.4            | 53             |
| 88  | Nanoengineered nonuniform strain in graphene using nanopillars. <i>Physical Review B</i> , <b>2012</b> , 86,                            | 3.3             | 49             |
| 87  | Defected graphene nanoribbons under axial compression. <i>Applied Physics Letters</i> , <b>2010</b> , 97, 153118                        | 3.4             | 47             |
| 86  | Thermal rippling behavior of graphane. <i>Physical Review B</i> , <b>2012</b> , 86,   | 3.3             | 46             |
| 85  | Lattice thermal properties of graphane: Thermal contraction, roughness, and heat capacity. <i>Physical Review B</i> , <b>2011</b> , 83, | 3.3             | 43             |

# (2014-2014)

| 84 | Stabilized silicene within bilayer graphene: A proposal based on molecular dynamics and density-functional tight-binding calculations. <i>Physical Review B</i> , <b>2014</b> , 89,     | 3.3                  | 42          |  |
|----|---|----------------------|-------------|--|
| 83 | AA-stacked bilayer square ice between graphene layers. <i>Physical Review B</i> , <b>2015</b> , 92,   | 3.3                  | 41          |  |
| 82 | Dependence of the shape of graphene nanobubbles on trapped substance. <i>Nature Communications</i> , <b>2017</b> , 8, 15844   | 17.4                 | 39          |  |
| 81 | Anomalous Dynamical Behavior of Freestanding Graphene Membranes. <i>Physical Review Letters</i> , <b>2016</b> , 117, 126801   | 7.4                  | 39          |  |
| 8o | Electronic structure of a hexagonal graphene flake subjected to triaxial stress. <i>Physical Review B</i> , <b>2013</b> , 88,   | 3.3                  | 39          |  |
| 79 | Linear reduction of stiffness and vibration frequencies in defected circular monolayer graphene. <i>Physical Review B</i> , <b>2010</b> , 81,   | 3.3                  | 39          |  |
| 78 | Rippling, buckling, and melting of single- and multilayer MoS2. <i>Physical Review B</i> , <b>2015</b> , 91,  | 3.3                  | 37          |  |
| 77 | Boron Nitride Monolayer: A Strain-Tunable Nanosensor. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 132   | 26 <del>3.</del> 832 | <b>63</b> 7 |  |
| 76 | Asymmetric simple exclusion process describing conflicting traffic flows. <i>Europhysics Letters</i> , <b>2007</b> , 80, 60002  | 1.6                  | 37          |  |
| 75 | Tuning the electronic properties of graphene@raphitic carbon nitride heterostructures and heterojunctions by using an electric field. <i>Physical Review B</i> , <b>2020</b> , 101,     | 3.3                  | 36          |  |
| 74 | Self-organized platinum nanoparticles on freestanding graphene. ACS Nano, 2014, 8, 2697-703   | 16.7                 | 36          |  |
| 73 | Induced polarization and electronic properties of carbon-doped boron nitride nanoribbons. <i>Physical Review B</i> , <b>2012</b> , 86,  | 3.3                  | 36          |  |
| 72 | Diffusive motion of C60 on a graphene sheet. <i>Physical Review E</i> , <b>2010</b> , 82, 051605  | 2.4                  | 34          |  |
| 71 | Thermal mirror buckling in freestanding graphene locally controlled by scanning tunnelling microscopy. <i>Nature Communications</i> , <b>2014</b> , 5, 4962                             | 17.4                 | 31          |  |
| 70 | Directed motion of C60 on a graphene sheet subjected to a temperature gradient. <i>Physical Review E</i> , <b>2011</b> , 83, 042601   | 2.4                  | 31          |  |
| 69 | Two-dimensional graphitic carbon nitrides: Strain-tunable ferromagnetic ordering. <i>Physical Review B</i> , <b>2020</b> , 101,   | 3.3                  | 30          |  |
| 68 | Electric-field-induced structural changes in water confined between two graphene layers. <i>Physical Review B</i> , <b>2016</b> , 94,   | 3.3                  | 28          |  |
| 67 | Electronic properties of graphene nano-flakes: energy gap, permanent dipole, termination effect, and Raman spectroscopy. <i>Journal of Chemical Physics</i> , <b>2014</b> , 140, 074304 | 3.9                  | 28          |  |

| 66 | Strain-engineered graphene through a nanostructured substrate. II. Pseudomagnetic fields. <i>Physical Review B</i> , <b>2012</b> , 85,   | 3.3  | 28 |
|----|--|------|----|
| 65 | Transport of hydrogen isotopes through interlayer spacing in van der Waals crystals. <i>Nature Nanotechnology</i> , <b>2018</b> , 13, 468-472  | 28.7 | 26 |
| 64 | Melting of graphene clusters. <i>Physical Review B</i> , <b>2013</b> , 87,   | 3.3  | 24 |
| 63 | Fast water flow through graphene nanocapillaries: A continuum model approach involving the microscopic structure of confined water. <i>Applied Physics Letters</i> , <b>2018</b> , 113, 083101 | 3.4  | 23 |
| 62 | Buckled circular monolayer graphene: a graphene nano-bowl. <i>Journal of Physics Condensed Matter</i> , <b>2011</b> , 23, 045002   | 1.8  | 23 |
| 61 | Reversible structural transition in nanoconfined ice. <i>Physical Review B</i> , <b>2017</b> , 95,   | 3.3  | 21 |
| 60 | Out-of-plane permittivity of confined water. <i>Physical Review E</i> , <b>2020</b> , 102, 022803  | 2.4  | 20 |
| 59 | Electro- and opto-mutable properties of MgO nanoclusters adsorbed on mono- and double-layer graphene. <i>Nanoscale</i> , <b>2017</b> , 9, 4205-4218  | 7.7  | 19 |
| 58 | Graphene ripples as a realization of a two-dimensional Ising model: A scanning tunneling microscope study. <i>Physical Review B</i> , <b>2015</b> , 91,  | 3.3  | 19 |
| 57 | Monolayer alkali and transition-metal monoxides: MgO, CaO, MnO, and NiO. <i>Physical Review B</i> , <b>2017</b> , 95,  | 3.3  | 19 |
| 56 | Spiral graphone and one-sided fluorographene nanoribbons. <i>Physical Review B</i> , <b>2013</b> , 87,   | 3.3  | 17 |
| 55 | Ground-state properties of a confined simple atom by C60fullerene. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , <b>2007</b> , 40, 1509-1521                            | 1.3  | 17 |
| 54 | Multilayer graphene, Moir[patterns, grain boundaries and defects identified by scanning tunneling microscopy on the m-plane, non-polar surface of SiC. <i>Carbon</i> , <b>2014</b> , 80, 75-81 | 10.4 | 16 |
| 53 | Graphene-silicene bilayer: A nanocapacitor with permanent dipole and piezoelectricity effect. <i>Physical Review B</i> , <b>2015</b> , 92,   | 3.3  | 16 |
| 52 | Graphene on hexagonal lattice substrate: Stress and pseudo-magnetic field. <i>Applied Physics Letters</i> , <b>2014</b> , 104, 173106  | 3.4  | 16 |
| 51 | Methane molecule over the defected and rippled graphene sheet. <i>Solid State Communications</i> , <b>2012</b> , 152, 1493-1496  | 1.6  | 16 |
| 50 | Effect of grain boundary on the buckling of graphene nanoribbons. <i>Applied Physics Letters</i> , <b>2012</b> , 100, 101905   | 3.4  | 16 |
| 49 | N-doped graphene: Polarization effects and structural properties. <i>Physical Review B</i> , <b>2016</b> , 93,   | 3.3  | 15 |

# (2021-2015)

| 48 | Diffusion of fluorine on and between graphene layers. Physical Review B, 2015, 91,  | 3.3            | 15 |
|----|---|----------------|----|
| 47 | Melting of Partially Fluorinated Graphene: From Detachment of Fluorine Atoms to Large Defects and Random Coils. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 4460-4464                           | 3.8            | 14 |
| 46 | Thermomechanical properties of graphene: valence force field model approach. <i>Journal of Physics Condensed Matter</i> , <b>2012</b> , 24, 175303  | 1.8            | 14 |
| 45 | The effects of temperature and vacancies on dynamics of crack in graphene sheet. <i>AIP Advances</i> , <b>2014</b> , 4, 057113  | 1.5            | 13 |
| 44 | Thermal activated rotation of graphene flake on graphene. 2D Materials, 2017, 4, 025015   | 5.9            | 12 |
| 43 | The different adsorption mechanism of methane molecule onto a boron nitride and a graphene flakes. <i>Journal of Applied Physics</i> , <b>2014</b> , 116, 153507  | 2.5            | 12 |
| 42 | Doping effect on the adsorption of NH3 molecule onto graphene quantum dot: From the physisorption to the chemisorption. <i>Journal of Applied Physics</i> , <b>2013</b> , 114, 124307                           | 2.5            | 12 |
| 41 | Trilayer Metal-Organic Frameworks as Multifunctional Electrocatalysts for Energy Conversion and Storage Applications <i>Journal of the American Chemical Society</i> , <b>2022</b> ,                            | 16.4           | 12 |
| 40 | Temperature distribution in graphene doped with nitrogen and graphene with grain boundary.<br>Journal of Molecular Graphics and Modelling, <b>2017</b> , 74, 100-104  | 2.8            | 11 |
| 39 | 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> , <b>2014</b> , 90, | 3.3            | 9  |
| 38 | Electronic, dielectric, and optical properties of two-dimensional and bulk ice: A multiscale simulation study. <i>Physical Review B</i> , <b>2020</b> , 101,  | 3.3            | 8  |
| 37 | Stochastic motion of noble gases on a graphene sheet. Computational Materials Science, 2010, 49, 839-8  | 8 <b>4</b> ,42 | 8  |
| 36 | Gas flow through atomic-scale apertures. Science Advances, 2020, 6,   | 14.3           | 8  |
| 35 | Self-Limiting Growth of Two-Dimensional Palladium between Graphene Oxide Layers. <i>Nano Letters</i> , <b>2019</b> , 19, 4678-4683  | 11.5           | 7  |
| 34 | Ionized water confined in graphene nanochannels. Physical Chemistry Chemical Physics, 2019, 21, 9285-   | 9395           | 7  |
| 33 | Electrostrictive behavior of confined water subjected to GPa pressure. <i>Physical Review B</i> , <b>2018</b> , 97,   | 3.3            | 7  |
| 32 | Monte Carlo simulation of size effects on thermal conductivity in a two-dimensional Ising system. <i>Physica A: Statistical Mechanics and Its Applications</i> , <b>2006</b> , 371, 424-432                     | 3.3            | 7  |
| 31 | The inhibition performance of quinoa seed on corrosion behavior of carbon steel in the HCl solution; theoretical and experimental evaluations. <i>Journal of Molecular Liquids</i> , <b>2021</b> , 335, 116183  | 6              | 7  |

| 30 | Slippage dynamics of confined water in graphene oxide capillaries. <i>Physical Review Materials</i> , <b>2018</b> , 2,   | 3.2                               | 6 |
|----|--|-----------------------------------|---|
| 29 | Molecular dynamics simulation of temperature profile in partially hydrogenated graphene and graphene with grain boundary. <i>Journal of Molecular Graphics and Modelling</i> , <b>2015</b> , 62, 38-42 | 2.8                               | 5 |
| 28 | Mechanical properties of twin graphene subjected to uniaxial stress by molecular dynamic simulation. <i>Materials Research Express</i> , <b>2019</b> , 6, 105611                                       | 1.7                               | 5 |
| 27 | Abnormal in-plane permittivity and ferroelectricity of confined water: From sub-nanometer channels to bulk. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 114503                             | 3.9                               | 5 |
| 26 | Breakdown of Universal Scaling for Nanometer-Sized Bubbles in Graphene. <i>Nano Letters</i> , <b>2021</b> , 21, 8103   | 3 <del>-8</del> 11 <del>9</del> 0 | 5 |
| 25 | Static flexural modes and piezoelectricity in 2D and layered crystals. <i>Physica Status Solidi (B): Basic Research</i> , <b>2016</b> , 253, 2311-2315   | 1.3                               | 4 |
| 24 | Partially hydrogenated and fluorinated graphene: Structure, roughness, and negative thermal expansion. <i>Physical Review B</i> , <b>2015</b> , 92,  | 3.3                               | 4 |
| 23 | Electric field effects on Nano-Scale bio-membrane of spherical cells. <i>Physica A: Statistical Mechanics and Its Applications</i> , <b>2009</b> , 388, 120-128  | 3.3                               | 4 |
| 22 | Ground state study of simple atoms within a nanoscale box. Solid State Communications, 2008, 145, 594  | -599                              | 4 |
| 21 | Van der Waals energy surface of a carbon nanotube sheet. <i>Solid State Communications</i> , <b>2012</b> , 152, 225-2  | 2306                              | 3 |
| 20 | Gas Permeability and Selectivity of a Porous WS2 Monolayer. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 25055-25066  | 3.8                               | 3 |
| 19 | Hydration effects and negative dielectric constant of nano-confined water between cation intercalated MXenes. <i>Nanoscale</i> , <b>2021</b> , 13, 922-929   | 7.7                               | 3 |
| 18 | Abnormal Dielectric Constant of Nanoconfined Water between Graphene Layers in the Presence of Salt. <i>Journal of Physical Chemistry B</i> , <b>2021</b> , 125, 1604-1610                              | 3.4                               | 3 |
| 17 | Large CO2 uptake on a monolayer of CaO. <i>Journal of Materials Chemistry A</i> , <b>2017</b> , 5, 2110-2114   | 13                                | 2 |
| 16 | Electric-field-induced emergent electrical connectivity in graphene oxide. <i>Physical Review B</i> , <b>2019</b> , 99,  | 3.3                               | 2 |
| 15 | Optoelectronic properties of confined water in angstrom-scale slits. <i>Physical Review B</i> , <b>2020</b> , 102,   | 3.3                               | 2 |
| 14 | The formation of Cr2O3 nanoclusters over graphene sheet and carbon nanotubes. <i>Chemical Physics Letters</i> , <b>2017</b> , 687, 188-193   | 2.5                               | 2 |
| 13 | Spatial design and control of graphene flake motion. <i>Physical Review B</i> , <b>2017</b> , 96,  | 3.3                               | 2 |

### LIST OF PUBLICATIONS

| 12 | Comment on "Irreversibility in response to forces acting on graphene sheets". <i>Physical Review Letters</i> , <b>2011</b> , 106, 209701; author reply 209702  | 7.4  | 2 |
|----|--|------|---|
| 11 | Enhanced roughness of lipid membranes caused by external electric fields. <i>Computational Materials Science</i> , <b>2007</b> , 41, 202-207   | 3.2  | 2 |
| 10 | Study of Hydrogen Molecule and Hydrogen Molecular Ion Confined in C60 Fullerene. <i>Journal of Computational and Theoretical Nanoscience</i> , <b>2008</b> , 5, 366-374                                | 0.3  | 2 |
| 9  | Unconventional two-dimensional vibrations of a decorated carbon nanotube under electric field: linking actuation to advanced sensing ability. <i>Scientific Reports</i> , <b>2017</b> , 7, 13481       | 4.9  | 1 |
| 8  | Evaluating gas permeance through graphene nanopores and porous 2D-membranes: A generalized approach. <i>Carbon Trends</i> , <b>2021</b> , 5, 100086  | 0    | 1 |
| 7  | Catalytic properties of cyclo-carbon clusters: An investigation on o2 activation and CO oxidation. <i>Surface Science</i> , <b>2022</b> , 720, 122050  | 1.8  | О |
| 6  | Oscillation in the electrical conductivity of a thick graphene oxide membrane. <i>Journal of Applied Physics</i> , <b>2021</b> , 129, 235105   | 2.5  | О |
| 5  | Tunable natural terahertz and mid-infrared hyperbolic plasmons in carbon phosphide. <i>Carbon</i> , <b>2021</b> , 178, 625-631   | 10.4 | O |
| 4  | Electronic Properties of Oxidized Graphene: Effects of Strain and an Electric Field on Flat Bands and the Energy Gap <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 66-74                | 6.4  | О |
| 3  | Effective potential of longitudinal interactions between microtubule protofilaments. <i>Physical Review E</i> , <b>2008</b> , 78, 011912   | 2.4  |   |
| 2  | Comment on A novel two-dimensional boron-carbon-nitride (BCN) monolayer: A first-principles insight[[J. Appl. Phys. 130, 114301 (2021)]. <i>Journal of Applied Physics</i> , <b>2022</b> , 131, 216101 | 2.5  |   |
| 1  | Simulative Molecular Modelling of MXene. <i>Engineering Materials</i> , <b>2022</b> , 109-138  | 0.4  |   |