# Javad Beheshtian

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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|---|---|---|---|
| 98 papers | 4,237 citations | 40 h-index | 63 g-index |
| 103 ext. papers | 4,687 ext. citations | 3.5 avg, IF | 5.95 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 98 | Electrodeposition of CoxNiVyOz Ternary Nanopetals on Bare and rGO-Coated Nickel Foam for High-Performance Supercapacitor Application. *Nanomaterials*, **2022**, 12, 1894 | 5.4 | 1 |
| 97 | A computational study on the BN and AlN nanocones as anode materials for K-ion batteries. *Applied Surface Science*, **2021**, 544, 148793 | 6.7 | 1 |
| 96 | A DFT study on the potential application of pristine, B and N doped carbon nanocones in potassium-ion batteries. *Journal of Molecular Modeling*, **2021**, 27, 168 | 2 | 2 |
| 95 | A computational study on the novel defects of graphene quantum dot as a promising anode material for sodium ion battery. *Materials Chemistry and Physics*, **2021**, 265, 124484 | 4.4 | 2 |
| 94 | Electronic, magnetic and optical properties of Fe-doped nano-BN sheet: DFT study. *Indian Journal of Physics*, **2021**, 95, 823-831 | 1.4 | 3 |
| 93 | Experimental and Theoretical Study of Porous Al2O3. *Transactions of the Indian Institute of Metals*, **2021**, 74, 381-386 | 1.2 | |
| 92 | Helium selectivity of H-, B-, N-, and F- doped nanoporous graphene membranes in the presence of natural gas: A density functional theory study. *Superlattices and Microstructures*, **2020**, 141, 106478 | 2.8 | 2 |
| 91 | The influence of Stone-Wales defects in nanographene on the performance of Na-ion batteries. *Journal of Molecular Graphics and Modelling*, **2020**, 98, 107578 | 2.8 | 5 |
| 90 | Electro-Optical Properties of Monolayer and Bilayer Pentagonal BN: First Principles Study. *Nanomaterials*, **2020**, 10, | 5.4 | 8 |
| 89 | Phase transition and mechanical properties of cesium bismuth silver halide double perovskites (CsAgBiX, X = Cl, Br, I): a DFT approach. *Physical Chemistry Chemical Physics*, **2020**, 22, 5959-5968 | 3.6 | 12 |
| 88 | Application of hexa-peri-hexabenzocoronene nanographene and its B, N, and Bn doped forms in Na-ion batteries: A density functional theory study. *Thin Solid Films*, **2020**, 704, 137979 | 2.2 | 3 |
| 87 | Hydrogenated graphene as an ultraviolet optomechanical sensor.. *RSC Advances*, **2020**, 10, 26197-26211 | 3.7 | 2 |
| 86 | Electronic and optical properties of vacancy and B, N, O and F doped graphene: DFT study. *Opto-electronics Review*, **2019**, 27, 130-136 | 2.4 | 16 |
| 85 | Ab Initio Study of Mono-Layer Graphene as an Electronical or Optical Sensor for Detecting B, N, O and F Atoms. *Journal of Electronic Materials*, **2019**, 48, 4265-4272 | 1.9 | 1 |
| 84 | Interfacial properties of water/heavy water layer encapsulate in bilayer graphene nanochannel and nanocapacitor. *Journal of Materials Science: Materials in Electronics*, **2019**, 30, 11964-11975 | 2.1 | 1 |
| 83 | Boron nitride nanochannels encapsulating a water/heavy water layer for energy applications.. *RSC Advances*, **2019**, 9, 5901-5907 | 3.7 | 2 |
| 82 | The electronic and optical properties of 3d transition metals doped silicene sheet: A DFT study. *Materials Research Express*, **2019**, 6, 126326 | 1.7 | 3 |

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| 81 | Ultrasonic route synthesis, characterization and electrochemical study of graphene oxide and reduced graphene oxide. *Research on Chemical Intermediates*, **2019**, 45, 487-505 | 2.8 | 13 |
| 80 | Natural pigments in dye-sensitized solar cell (DSSC): a DFT-TDDFT study. *Journal of the Iranian Chemical Society*, **2019**, 16, 795-805 | 2 | 21 |
| 79 | Nanoscale investigation of the influence of water on the elastic properties of C□H gel by molecular simulation. *Proceedings of the Institution of Mechanical Engineers, Part L: Journal of Materials: Design and Applications*, **2019**, 233, 1295-1306 | 1.3 | 2 |
| 78 | Effect of nitrogen doping on electronic and optical properties of ZnO sheet: DFT+U study. *Computational Condensed Matter*, **2018**, 15, 1-6 | 1.7 | 5 |
| 77 | First-Principles Study of Water Nanotubes Captured Inside Carbon/Boron Nitride Nanotubes. *Langmuir*, **2018**, 34, 11176-11187 | 4 | 14 |
| 76 | Experimental and Theoretical Study of Enhanced Photocatalytic Activity of Mg-Doped ZnO NPs and ZnO/rGO Nanocomposites. *Chemistry - an Asian Journal*, **2018**, 13, 194-203 | 4.5 | 67 |
| 75 | Toxic CO detection by Li-encapsulated fullerene-like BeO. *Structural Chemistry*, **2018**, 29, 231-241 | 1.8 | 6 |
| 74 | Synthesis of undoped and Fe nanoparticles doped SnO2 nanostructure: study of structural, optical and electrocatalytic properties. *Journal of Materials Science: Materials in Electronics*, **2017**, 28, 7568-7574 | 2.1 | 7 |
| 73 | Reversible structural transition in nanoconfined ice. *Physical Review B*, **2017**, 95, | 3.3 | 21 |
| 72 | Voltammetric Sensor Based on Fe-doped ZnO and TiO2 Nanostructures-modified Carbon-paste Electrode for Determination of Levodopa. *Journal of Electronic Materials*, **2017**, 46, 5657-5663 | 1.9 | 6 |
| 71 | Effects of functionalization and side defects on single-photon emission in boron nitride quantum dots. *Physical Review B*, **2017**, 96, | 3.3 | 15 |
| 70 | Microporous titania□silica nanocomposite catalyst-adsorbent for ultra-deep oxidative desulfurization. *Applied Catalysis B: Environmental*, **2016**, 180, 65-77 | 21.8 | 128 |
| 69 | Van der Waals pressure and its effect on trapped interlayer molecules. *Nature Communications*, **2016**, 7, 12168 | 17.4 | 91 |
| 68 | Selective separation behavior of graphene flakes in interaction with halide anions in the presence of an external electric field. *Physical Chemistry Chemical Physics*, **2016**, 18, 7293-9 | 3.6 | 12 |
| 67 | Hydrogen storage by BeO nano-cage: A DFT study. *Applied Surface Science*, **2016**, 368, 76-81 | 6.7 | 28 |
| 66 | Highly sensitive and selective ethanol and acetone gas sensors by adding some dopants (Mn, Fe, Co, Ni) onto hexagonal ZnO plates. *RSC Advances*, **2016**, 6, 7838-7845 | 3.7 | 57 |
| 65 | Electrochemical and DFT study of an anticancer and active anthelmintic drug at carbon nanostructured modified electrode. *Materials Science and Engineering C*, **2016**, 69, 1345-53 | 8.3 | 23 |
| 64 | Preparation of Cu2O nanostructures by changing reducing agent and their optical properties. *Materials Letters*, **2015**, 153, 1-4 | 3.3 | 22 |

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| 63 | Theoretical prediction of silicene as a new candidate for the anode of lithium-ion batteries. *Physical Chemistry Chemical Physics*, **2015**, 17, 29689-96 | 3.6 | 48 |
| 62 | Highly active Fe2O3-doped TiO2 photocatalyst for degradation of trichloroethylene in air under UV and visible light irradiation: Experimental and computational studies. *Applied Catalysis B: Environmental*, **2015**, 165, 209-221 | 21.8 | 103 |
| 61 | Graphene-silicene bilayer: A nanocapacitor with permanent dipole and piezoelectricity effect. *Physical Review B*, **2015**, 92, | 3.3 | 16 |
| 60 | Synthesis, identification, crystal structure and theoretical study of a Ce(IV) complex. *Journal of the Iranian Chemical Society*, **2014**, 11, 1353-1361 | 2 | 3 |
| 59 | Experimental and theoretical study of CO adsorption on the surface of single phase hexagonally plate ZnO. *Applied Surface Science*, **2014**, 315, 8-15 | 6.7 | 12 |
| 58 | Preparation of uniform 2D ZnO nanostructures by the ionic liquid-assisted sonochemical method and their optical properties. *Ceramics International*, **2014**, 40, 7769-7774 | 5.1 | 25 |
| 57 | Theoretical investigation of azo dyes adsorbed on cellulose fibers: 2. Spectroscopic study. *Journal of the Iranian Chemical Society*, **2014**, 11, 111-121 | 2 | 1 |
| 56 | Density-functional calculations of HCN adsorption on the pristine and Si-doped graphynes. *Structural Chemistry*, **2014**, 25, 1-7 | 1.8 | 62 |
| 55 | Theoretical investigation of azo dyes adsorbed on cellulose fibers: 1. Electronic and bonding structures. *Journal of the Iranian Chemical Society*, **2013**, 10, 985-999 | 2 | 1 |
| 54 | Functionalization of BN nanosheet with N2H4 may be feasible in the presence of Stone□Wales defect. *Structural Chemistry*, **2013**, 24, 1565-1570 | 1.8 | 78 |
| 53 | Formaldehyde adsorption on the interior and exterior surfaces of CN nanotubes. *Structural Chemistry*, **2013**, 24, 1331-1337 | 1.8 | 33 |
| 52 | Ab initio study of NH3 and H2O adsorption on pristine and Na-doped MgO nanotubes. *Structural Chemistry*, **2013**, 24, 165-170 | 1.8 | 76 |
| 51 | Sensing behavior of Al-rich AlN nanotube toward hydrogen cyanide. *Journal of Molecular Modeling*, **2013**, 19, 2197-203 | 2 | 58 |
| 50 | Computational study of ammonia adsorption on the perfect and rippled graphene sheet. *Physica B: Condensed Matter*, **2013**, 429, 52-56 | 2.8 | 11 |
| 49 | DFT study on the functionalization of a BN nanotube with sulfamide. *Applied Surface Science*, **2013**, 266, 182-187 | 6.7 | 78 |
| 48 | A DFT study on the functionalization of a BN nanosheet with PCX, (PC=phenyl carbamate, X=OCH3, CH3, NH2, NO2 and CN). *Applied Surface Science*, **2013**, 268, 436-441 | 6.7 | 100 |
| 47 | Doping effect on the adsorption of NH3 molecule onto graphene quantum dot: From the physisorption to the chemisorption. *Journal of Applied Physics*, **2013**, 114, 124307 | 2.5 | 12 |
| 46 | Hydrogen dissociation on diene-functionalized carbon nanotubes. *Journal of Molecular Modeling*, **2013**, 19, 255-61 | 2 | 63 |

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| 45 | Carbon nanotube functionalization with carboxylic derivatives: a DFT study. *Journal of Molecular Modeling*, **2013**, 19, 391-6 | 2 | 58 |
| 44 | Arsenic interactions with a fullerene-like BN cage in the vacuum and aqueous phase. *Journal of Molecular Modeling*, **2013**, 19, 833-7 | 2 | 26 |
| 43 | Nitrous oxide adsorption on pristine and Si-doped AlN nanotubes. *Journal of Molecular Modeling*, **2013**, 19, 943-9 | 2 | 26 |
| 42 | Sensing behavior of Al and Si doped BC3 graphenes to formaldehyde. *Sensors and Actuators B: Chemical*, **2013**, 181, 829-834 | 8.5 | 158 |
| 41 | Spiral graphone and one-sided fluorographene nanoribbons. *Physical Review B*, **2013**, 87, | 3.3 | 17 |
| 40 | Ammonia monitoring by carbon nitride nanotubes: A density functional study. *Thin Solid Films*, **2013**, 534, 650-654 | 2.2 | 62 |
| 39 | Exohedral and endohedral adsorption of alkaline earth cations in BN nanocluster. *Journal of Molecular Modeling*, **2013**, 19, 1445-50 | 2 | 27 |
| 38 | Theoretical study on the functionalization of BCN nanotube with amino groups. *Journal of Molecular Modeling*, **2013**, 19, 2211-6 | 2 | 10 |
| 37 | Boron Nitride Monolayer: A Strain-Tunable Nanosensor. *Journal of Physical Chemistry C*, **2013**, 117, 13261-13267 | 3.8 | 37 |
| 36 | Carbon nitride nanotube as a sensor for alkali and alkaline earth cations. *Applied Surface Science*, **2013**, 264, 699-706 | 6.7 | 80 |
| 35 | AlN nanotube as a potential electronic sensor for nitrogen dioxide. *Microelectronics Journal*, **2012**, 43, 452-455 | 1.8 | 84 |
| 34 | Nitrate adsorption by carbon nanotubes in the vacuum and aqueous phase. *Monatshefte Fü Chemie*, **2012**, 143, 1623-1626 | 1.4 | 65 |
| 33 | Electronic sensor for sulfide dioxide based on AlN nanotubes: a computational study. *Journal of Molecular Modeling*, **2012**, 18, 4745-50 | 2 | 70 |
| 32 | Induced polarization and electronic properties of carbon-doped boron nitride nanoribbons. *Physical Review B*, **2012**, 86, | 3.3 | 36 |
| 31 | A first-principles study of H2S adsorption and dissociation on the AlN nanotube. *Physica E: Low-Dimensional Systems and Nanostructures*, **2012**, 44, 1963-1968 | 3 | 83 |
| 30 | Theoretical study of CO adsorption on the surface of BN, AlN, BP and AlP nanotubes. *Surface Science*, **2012**, 606, 981-985 | 1.8 | 125 |
| 29 | Adsorption and dissociation of Cl2 molecule on ZnO nanocluster. *Applied Surface Science*, **2012**, 258, 8171-8176 | 6.7 | 95 |
| 28 | Functionalization of [60] fullerene with butadienes: A DFT study. *Applied Surface Science*, **2012**, 258, 8980-8984 | 6.7 | 55 |

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| 27 | Quantum chemical study of fluorinated AlN nano-cage. *Applied Surface Science*, **2012**, 259, 631-636 | 6.7 | 86 |
| 26 | Selective function of Al12N12 nano-cage towards NO and CO molecules. *Computational Materials Science*, **2012**, 62, 71-74 | 3.2 | 113 |
| 25 | Theoretical investigation of C60 fullerene functionalization with tetrazine. *Computational and Theoretical Chemistry*, **2012**, 992, 164-167 | 2 | 61 |
| 24 | Theoretical study of hydrogen adsorption on the B12P12 fullerene-like nanocluster. *Computational Materials Science*, **2012**, 54, 115-118 | 3.2 | 83 |
| 23 | Adsorption of Na, Mg, and Al atoms on BN nanotubes. *Thin Solid Films*, **2012**, 526, 139-142 | 2.2 | 11 |
| 22 | Detection of phosgene by Sc-doped BN nanotubes: A DFT study. *Sensors and Actuators B: Chemical*, **2012**, 171-172, 846-852 | 8.5 | 240 |
| 21 | Interaction of small molecules (NO, H2, N2, and CH4) with BN nanocluster surface. *Structural Chemistry*, **2012**, 23, 1567-1572 | 1.8 | 86 |
| 20 | Co-adsorption of CO molecules at the open ends of MgO nanotubes. *Structural Chemistry*, **2012**, 23, 1981-1986 | 1.8 | 18 |
| 19 | A theoretical study of CO adsorption on aluminum nitride nanotubes. *Structural Chemistry*, **2012**, 23, 653-657 | 1.8 | 74 |
| 18 | Benchmarking of ONIOM method for the study of NH3 dissociation at open ends of BNNTs. *Journal of Molecular Modeling*, **2012**, 18, 1729-34 | 2 | 71 |
| 17 | The H2 dissociation on the BN, AlN, BP and AlP nanotubes: a comparative study. *Journal of Molecular Modeling*, **2012**, 18, 2343-8 | 2 | 80 |
| 16 | A comparative study on the B12N12, Al12N12, B12P12 and Al12P12 fullerene-like cages. *Journal of Molecular Modeling*, **2012**, 18, 2653-8 | 2 | 129 |
| 15 | B12N12 Nano-cage as Potential Sensor for NO2 Detection. *Chinese Journal of Chemical Physics*, **2012**, 25, 60-64 | 0.9 | 100 |
| 14 | The Alkali Metal Interactions with MgO Nanotubes. *Bulletin of the Korean Chemical Society*, **2012**, 33, 1925-1928 | 1.2 | 14 |
| 13 | Toxic CO detection by B12N12 nanocluster. *Microelectronics Journal*, **2011**, 42, 1400-1403 | 1.8 | 103 |
| 12 | Computational study of CO and NO adsorption on magnesium oxide nanotubes. *Physica E: Low-Dimensional Systems and Nanostructures*, **2011**, 44, 546-549 | 3 | 88 |
| 11 | Chemisorption of NH3 at the open ends of boron nitride nanotubes: a DFT study. *Structural Chemistry*, **2011**, 22, 183-188 | 1.8 | 84 |
| 10 | The effect of surface curvature of aluminum nitride nanotubes on the adsorption of NH3. *Structural Chemistry*, **2011**, 22, 1261-1265 | 1.8 | 63 |

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| 9 | Computational study on the characteristics of the interaction in linear urea clusters. *International Journal of Quantum Chemistry*, **2011**, 111, 3184-3195 | 2.1 | 36 |
| 8 | Photo-oxidation of phenylazonaphthol dyes and their reactivity analysis in the gas phase and adsorbed on cellulose fibers states using DFT and TD-DFT. *Dyes and Pigments*, **2011**, 89, 16-22 | 4.6 | 7 |
| 7 | Interaction of NH3 with aluminum nitride nanotube: Electrostatic vs. covalent. *Physica E: Low-Dimensional Systems and Nanostructures*, **2011**, 43, 1717-1719 | 3 | 76 |
| 6 | DFT study of NH3(H2O)n=0,1,2,3 complex adsorption on the (8, 0) single-walled carbon nanotube. *Computational Materials Science*, **2010**, 48, 655-657 | 3.2 | 11 |
| 5 | A computational study of water adsorption on boron nitride nanotube. *Structural Chemistry*, **2010**, 21, 903-908 | 1.8 | 33 |
| 4 | DFT study of NH3 adsorption on the (5,0), (8,0), (5,5) and (6,6) single-walled carbon nanotubes. Calculated binding energies, NMR and NQR parameters. *Physica B: Condensed Matter*, **2010**, 405, 1455-1460 | 2.8 | 32 |
| 3 | A density functional study of 15N chemical shielding tensors in quinolines. *Chemical Physics Letters*, **2009**, 476, 196-200 | 2.5 | 7 |
| 2 | 15N CHEMICAL SHIFT CALCULATIONS AND NATURAL BONDING ORBITAL ANALYSES OF (BENZAMIDE)n = 1 - 6 CLUSTERS. *Journal of Theoretical and Computational Chemistry*, **2009**, 08, 973-982 | 1.8 | 2 |
| 1 | Theoretical 14N nuclear quadrupole resonance parameters for sulfa drugs: sulfamerazine and sulfathiazole. *Journal of Molecular Graphics and Modelling*, **2008**, 27, 326-31 | 2.8 | 29 |