# Fernando Sato

List of Publications by Year
in descending order

| # | Article | IF | Citations |
| --- | --- | --- | --- |
| 1 | Tunable and sizeable band gaps in strained SiC3/hBN vdW heterostructures: A potential replacement for graphene in future nanoelectronics. Computational Materials Science, 2021, 188, 110233. | 3.0 | 8 |
| 2 | Magnetic characterization, electronic structure and vibrational properties of (NH4)2ÂM(SO4)2Â·6H2O (M=Mn, Ni) crystals. Solid State Communications, 2021, 334-335, 114384. | 1.9 | 3 |
| 3 | Experimental and theoretical study of solvent effect in graphene oxide. Journal of Molecular Liquids, 2021, 342, 117429. | 4.9 | 3 |
| 4 | Probing ring contraction and decarboxylation of Rhodizonate and the influence of Cu (II) using surfaceâ€enhanced Raman Scattering. Journal of Raman Spectroscopy, 2020, 51, 256-263. | 2.5 | 3 |
| 5 | Graphene oxide in water: a systematic computational experimental study. Graphene Technology, 2020, 5, 1-8. | 1.9 | 3 |
| 6 | Electronic properties of substitutional impurities in graphenelike <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math> , <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>t</mml:mi><mml:mi>g</mml:mi><mml:mtext>â^'</mml:r mathvariant="normal">C</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant | 3.2 | 11 |
| 7 | Origin of optical bandgap fluctuations in graphene oxide. European Physical Journal B, 2020, 93, 1. | 1.5 | 11 |
| 8 | Traps for pinning and scattering of antiferromagnetic skyrmions via magnetic properties engineering. Journal of Applied Physics, 2020, 127, . | 2.5 | 11 |
| 9 | Suppression of the skyrmion Hall effect in planar nanomagnets by the magnetic properties engineering: Skyrmion transport on nanotracks with magnetic strips. Journal of Magnetism and Magnetic Materials, 2020, 504, 166655. | 2.3 | 21 |
| 10 | Exotic impurity-induced states in single-layer h -BN: The role of sublattice structure and intervalley interactions. Physical Review B, 2019, 100, . | 3.2 | 6 |
| 11 | Tunable optoelectronic properties in h-BP/h-BAs bilayers: The effect of an external electrical field. Applied Surface Science, 2019, 493, 308-319. | 6.1 | 23 |
| 12 | Investigation of domain wall pinning by square anti-notches and its application in three terminals MRAM. Applied Physics Letters, 2019, 114, . | 3.3 | 11 |
| 13 | Non-trivial band gaps and charge transfer in Janus-like functionalized bilayer boron arsenide. Computational Materials Science, 2019, 170, 109186. | 3.0 | 4 |
| 14 | Theoretical characterization of hexagonal 2D Be<sub>3</sub>N<sub>2</sub> monolayers. New Journal of Chemistry, 2019, 43, 2933-2941. | 2.8 | 20 |
| 15 | Coupled cluster investigation of the interaction of beryllium, magnesium, and calcium with pyridine: Implications for the adsorption on nitrogen-doped graphene. Computational and Theoretical Chemistry, 2019, 1150, 57-62. | 2.5 | 12 |
| 16 | Monolayer boronâ€arsenide as a perfect anode for alkaliâ€based batteries with large storage capacities and fast mobilities. International Journal of Quantum Chemistry, 2019, 119, e25975. | 2.0 | 15 |
| 17 | High-Frequency Oscillator Based on Nano Graphene. Brazilian Journal of Physics, 2019, 49, 488-493. | 1.4 | 2 |
| 18 | Electronic properties and vibrational spectra of (NH4)2Mâ€³(SO4)2Â·6H2O (Mâ€¯=â€¯Ni, Cu) Tutton's salt: DFT and experimental study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 218, 281-292. | 3.9 | 16 |

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|---|---|---|---|
| 19 | Modeling a Hypothetical Zombie Outbreak Can Save Us from Real-World Monsters. Mathematical Intelligencer, 2019, 41, 72-79. | 0.2 | 0 |
| 20 | DFT calculations on the structural and electronic properties of vacancy effects in the silicon nanowires. European Physical Journal B, 2019, 92, 1. | 1.5 | 2 |
| 21 | Building traps for skyrmions by the incorporation of magnetic defects into nanomagnets: Pinning and scattering traps by magnetic properties engineering. Journal of Magnetism and Magnetic Materials, 2019, 480, 171-185. | 2.3 | 24 |
| 22 | Theoretical investigation of various aspects of two dimensional holey boroxine, B<sub>3</sub>O<sub>3</sub>. RSC Advances, 2019, 9, 37526-37536. | 3.6 | 21 |
| 23 | Adsorption and diffusion of alkaliâ€atoms (Li, Na, and K) on BeN dual doped graphene. International Journal of Quantum Chemistry, 2019, 119, e25900. | 2.0 | 16 |
| 24 | Hexagonal boron phosphide as a potential anode nominee for alkali-based batteries: A multi-flavor DFT study. Applied Surface Science, 2019, 471, 134-141. | 6.1 | 49 |
| 25 | Exploring the effect of substitutional doping on the electronic properties of graphene oxide. Journal of Materials Science, 2018, 53, 7516-7526. | 3.7 | 9 |
| 26 | Depinning of the transverse domain wall trapped at magnetic impurities patterned in planar nanowires: Control of the wall motion using low-intensity and short-duration current pulses. Journal of Magnetism and Magnetic Materials, 2018, 451, 639-646. | 2.3 | 10 |
| 27 | Theoretical evaluation of chemical substitutions along the main chain of poly(3â€hexylthienyleneâ€vinylene) for solar cell applications. Polymer International, 2018, 67, 197-203. | 3.1 | 2 |
| 28 | Adsorption of Sodium on Doped Graphene: A vdW-DF Study. Current Graphene Science, 2018, 2, 35-44. | 0.5 | 7 |
| 29 | Unusual Enhancement of the Adsorption Energies of Sodium and Potassium in Sulfurâˆ’Nitrogen and Siliconâˆ’Boron Codoped Graphene. ACS Omega, 2018, 3, 15821-15828. | 3.5 | 15 |
| 30 | Hydrogenation and Fluorination of 2D Boron Phosphide and Boron Arsenide: A Density Functional Theory Investigation. ACS Omega, 2018, 3, 16416-16423. | 3.5 | 38 |
| 31 | Effects of Mechanical Stretching on the Properties of Conjugated Polymers: Case Study for MEHâ€PPV and P3HT Oligomers. Journal of Polymer Science, Part B: Polymer Physics, 2018, 56, 1413-1426. | 2.1 | 11 |
| 32 | Modeling surface energy in porous metallic nanostructures. European Physical Journal B, 2018, 91, 1. | 1.5 | 2 |
| 33 | The role of sulfate in the chemical synthesis of graphene oxide. Materials Chemistry and Physics, 2018, 215, 203-210. | 4.0 | 12 |
| 34 | First-principles study of dual-doped graphene: towards promising anode materials for Li/Na-ion batteries. New Journal of Chemistry, 2018, 42, 10842-10851. | 2.8 | 44 |
| 35 | Coupled cluster and density functional investigation of the neutral sodium-benzene and potassium-benzene complexes. Chemical Physics Letters, 2018, 706, 343-347. | 2.6 | 11 |
| 36 | Tripleâ€Doped Monolayer Graphene with Boron, Nitrogen, Aluminum, Silicon, Phosphorus, and Sulfur. ChemPhysChem, 2017, 18, 1864-1873. | 2.1 | 49 |

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|---|---|---|---|
| 37 | Reduced graphene oxide prepared at low temperature thermal treatment as transparent conductors for organic electronic applications. Organic Electronics, 2017, 49, 165-173. | 2.6 | 31 |
| 38 | Rectangular and hexagonal doping of graphene with B, N, and O: a DFT study. RSC Advances, 2017, 7, 16064-16068. | 3.6 | 26 |
| 39 | Study on the coherence degree of magnetization reversal in Permalloy single-domain nano-ellipses. Journal of Magnetism and Magnetic Materials, 2017, 426, 396-404. | 2.3 | 2 |
| 40 | Beryllium doped graphene as an efficient anode material for lithium-ion batteries with significantly huge capacity: A DFT study. Applied Materials Today, 2017, 9, 333-340. | 4.3 | 84 |
| 41 | Structural, electronic, and magnetic properties of non-planar doping of BeO in graphene: a DFT study. New Journal of Chemistry, 2017, 41, 10780-10789. | 2.8 | 7 |
| 42 | Decreasing the size limit for a stable magnetic vortex in modified permalloy nanodiscs. Journal of Magnetism and Magnetic Materials, 2017, 443, 252-260. | 2.3 | 5 |
| 43 | Triple-Doped Monolayer Graphene with Boron, Nitrogen, Aluminum, Silicon, Phosphorus, and Sulfur. ChemPhysChem, 2017, 18, 1854-1854. | 2.1 | 3 |
| 44 | Vibrational spectroscopy for milk fat quantification: line shape analysis of the Raman and infrared spectra. Journal of Raman Spectroscopy, 2016, 47, 692-698. | 2.5 | 19 |
| 45 | Enhancement of nonlinear optical properties of graphene oxide-based structures: pushâ€“pull models. RSC Advances, 2016, 6, 94437-94450. | 3.6 | 15 |
| 46 | Structural and vibrational study of graphene oxide via coronene based models: theoretical and experimental results. Materials Research Express, 2016, 3, 055020. | 1.6 | 18 |
| 47 | Magnetization reversal of the transverse domain wall confined between two clusters of magnetic impurities in a ferromagnetic planar nanowire. Journal of Magnetism and Magnetic Materials, 2016, 419, 37-42. | 2.3 | 10 |
| 48 | Theoretical study of nonlinear optical properties of cobalt bis (dicarbollide) derivatives: the effect of substituents. Theoretical Chemistry Accounts, 2015, 134, 1. | 1.4 | 4 |
| 49 | Position of the transverse domain wall controlled by magnetic impurities in rectangular magnetic nanowires. Journal of Applied Physics, 2014, 115, . | 2.5 | 7 |
| 50 | Substituent effects on molecular properties of dicarba-closo-dodecarborane derivatives. Journal of Molecular Modeling, 2014, 20, 2275. | 1.8 | 5 |
| 51 | Dynamics of the vortex core in magnetic nanodisks with a ring of magnetic impurities. Applied Physics Letters, 2012, 101, . | 3.3 | 24 |
| 52 | The influence of magnetic impurities in the vortex core dynamics in magnetic nano-disks. Journal of Magnetism and Magnetic Materials, 2012, 324, 3083-3086. | 2.3 | 15 |
| 53 | van der Waals potential barrier for cobaltocene encapsulation into single-walled carbon nanotubes: classical molecular dynamics andab initiostudy. Molecular Simulation, 2011, 37, 746-751. | 2.0 | 1 |
| 54 | The First Molecular Wheel: A Theoretical Investigation. Materials Research Society Symposia Proceedings, 2011, 1286, 44. | 0.1 | 0 |

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| 55 | Adsorption configuration effects on the surface diffusion of large organic molecules: The case of Violet Lander. Journal of Chemical Physics, 2010, 133, 224702. | 3.0 | 3 |
| 56 | Temperature effects on the atomic arrangement and conductance of atomic-size gold nanowires generated by mechanical stretching. Nanotechnology, 2010, 21, 485702. | 2.6 | 18 |
| 57 | Observation of the smallest metal nanotube with a square cross-section. Nature Nanotechnology, 2009, 4, 149-152. | 31.5 | 50 |
| 58 | New Insights on the Growth of Anisotropic Nanoparticles from Total Energy Calculations. Journal of Physical Chemistry C, 2009, 113, 11976-11979. | 3.1 | 4 |
| 59 | Defects in Graphene-Based Twisted Nanoribbons: Structural, Electronic, and Optical Properties. Langmuir, 2009, 25, 4751-4759. | 3.5 | 26 |
| 60 | C<sub>60</sub>-derived nanobaskets: stability, vibrational signatures, and molecular trapping. Nanotechnology, 2009, 20, 395701. | 2.6 | 8 |
| 61 | Designing conducting polymers using bioinspired ant algorithms. Chemical Physics Letters, 2008, 453, 290-295. | 2.6 | 12 |
| 62 | MÃ¶bius and twisted graphene nanoribbons: Stability, geometry, and electronic properties. Journal of Chemical Physics, 2008, 128, 164719. | 3.0 | 54 |
| 63 | Size Limit of Defect Formation in Pyramidal Pt Nanocontacts. Physical Review Letters, 2007, 99, 255501. | 7.8 | 16 |
| 64 | Experimental realization of suspended atomic chains composed of different atomic species. Nature Nanotechnology, 2006, 1, 182-185. | 31.5 | 95 |
| 65 | Computer simulations of gold nanowire formation: the role of outlayer atoms. Applied Physics A: Materials Science and Processing, 2005, 81, 1527-1531. | 2.3 | 31 |
| 66 | Prediction of Ordered Phases of Encapsulated C60, C70, and C78Inside Carbon Nanotubes. Nano Letters, 2005, 5, 349-355. | 9.1 | 85 |
| 67 | Lock-and-key effect in the surface diffusion of large organic molecules probed by STM. Nature Materials, 2004, 3, 779-782. | 27.5 | 116 |
| 68 | On the Structural and Stability Features of Linear Atomic Suspended Chains Formed from Gold Nanowires Stretching. Nano Letters, 2004, 4, 1187-1191. | 9.1 | 106 |
| 69 | Indication of Unusual Pentagonal Structures in Atomic-Size Cu Nanowires. Physical Review Letters, 2004, 93, 126103. | 7.8 | 105 |