# Qingyang Fan

List of Publications by Year
in descending order

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|---|---|---|---|
| 69<br>papers | 1,677<br>citations | 257450<br>24<br>h-index | 330143<br>37<br>g-index |
| 70<br>all docs | 70<br>docs citations | 70<br>times ranked | 543<br>citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Elastic and electronic properties of Pbca-BN: First-principles calculations. Computational Materials Science, 2014, 85, 80-87. | 3.0 | 114 |
| 2 | Structural, mechanical, and electronic properties of P3m1-BCN. Journal of Physics and Chemistry of Solids, 2015, 79, 89-96. | 4.0 | 79 |
| 3 | A hybrid niobium-based oxide with bio-based porous carbon as an efficient electrocatalyst in photovoltaics: a general strategy for understanding the catalytic mechanism. Journal of Materials Chemistry A, 2019, 7, 14864-14875. | 10.3 | 74 |
| 4 | PBCFâ€Graphene: A 2D Sp<sup>2</sup> Hybridized Honeycomb Carbon Allotrope with a Direct Band Gap. ChemNanoMat, 2020, 6, 139-147. | 2.8 | 54 |
| 5 | Enhanced direct interspecies electron transfer with transition metal oxide accelerants in anaerobic digestion. Bioresource Technology, 2021, 320, 124294. | 9.6 | 52 |
| 6 | Two novel silicon phases with direct band gaps. Physical Chemistry Chemical Physics, 2016, 18, 12905-12913. | 2.8 | 50 |
| 7 | Five carbon allotropes from Squaroglitter structures. Computational Materials Science, 2020, 178, 109634. | 3.0 | 49 |
| 8 | IIIâ€Nitride Polymorphs: XN (X=Al, Ga, In) in the Pnma Phase. Chemistry - A European Journal, 2018, 24, 17280-17287. | 3.3 | 46 |
| 9 | tâ€Si<sub>64</sub>: A Novel Silicon Allotrope. ChemPhysChem, 2019, 20, 128-133. | 2.1 | 45 |
| 10 | Novel silicon allotropes: Stability, mechanical, and electronic properties. Journal of Applied Physics, 2015, 118, . | 2.5 | 44 |
| 11 | Stability, mechanical, anisotropic and electronic properties of oP8 carbon: A superhard carbon allotrope in orthorhombic phase. Journal of Solid State Chemistry, 2021, 294, 121894. | 2.9 | 42 |
| 12 | Two novel superhard carbon allotropes with honeycomb structures. Journal of Applied Physics, 2019, 126, . | 2.5 | 41 |
| 13 | Two-dimensional carbon allotropes with tunable direct band gaps and high carrier mobility. Applied Surface Science, 2021, 537, 147885. | 6.1 | 39 |
| 14 | Prediction of novel phase of silicon and Siâ€“Ge alloys. Journal of Solid State Chemistry, 2016, 233, 471-483. | 2.9 | 37 |
| 15 | Two orthorhombic superhard carbon allotropes: C16 and C24. Diamond and Related Materials, 2021, 116, 108426. | 3.9 | 35 |
| 16 | Two Novel C3N4 Phases: Structural, Mechanical and Electronic Properties. Materials, 2016, 9, 427. | 2.9 | 34 |
| 17 | An orthorhombic superhard carbon allotrope: Pmma C24. Journal of Solid State Chemistry, 2021, 300, 122260. | 2.9 | 33 |
| 18 | Theoretical investigations of group IV alloys in the Lonsdaleite phase. Journal of Materials Science, 2018, 53, 2785-2801. | 3.7 | 31 |

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|---|---|---|---|
| 19 | Physical properties of a novel microporous carbon material. Diamond and Related Materials, 2020, 106, 107831. | 3.9 | 31 |
| 20 | Penta-C20: A Superhard Direct Band Gap Carbon Allotrope Composed of Carbon Pentagon. Materials, 2020, 13, 1926. | 2.9 | 31 |
| 21 | Mechanical and electronic properties of Si, Ge and their alloys in P42/mnm structure. Materials Science in Semiconductor Processing, 2016, 43, 187-195. | 4.0 | 29 |
| 22 | Two novel Ge phases and their Si Ge alloys with excellent electronic and optical properties. Materials and Design, 2017, 132, 539-551. | 7.0 | 27 |
| 23 | Si96: A New Silicon Allotrope with Interesting Physical Properties. Materials, 2016, 9, 284. | 2.9 | 26 |
| 24 | Theoretical investigations of Ge1â^'xSn x alloys (xâ€‰=â€‰0, 0.333, 0.667, 1) in P42/ncm phase. Journal of Materials Science, 2018, 53, 9611-9626. | 3.7 | 26 |
| 25 | P63/mmc-Ge and their Siâ€“Ge alloys with a mouldable direct band gap. Semiconductor Science and Technology, 2020, 35, 055012. | 2.0 | 26 |
| 26 | Elastic and electronic properties of Imm2- and I<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:mover accent="true"><mml:mrow><mml:mn>4</mml:mn></mml:mrow><mml:mrow><mml:mo>Â¯</mml:mo></mml:mrow></mml:mover></m Computational Materials Science, 2015, 97, 6-13. | 3.0 | 25 |
| 27 | Physical Properties of XN (X = B, Al, Ga, In) in the Pmâ^'3n phase: First-Principles Calculations. Materials, 2020, 13, 1280. | 2.9 | 25 |
| 28 | Physical properties of group 14 semiconductor alloys in orthorhombic phase. Journal of Applied Physics, 2019, 126, 045709. | 2.5 | 24 |
| 29 | Three-dimensional metallic carbon allotropes with superhardness. Nanotechnology Reviews, 2021, 10, 1266-1276. | 5.8 | 24 |
| 30 | Physical properties of group 14 elements in P2/m phase. Journal of Solid State Chemistry, 2022, 305, 122641. | 2.9 | 24 |
| 31 | All sp2 hybridization BN polymorphs with wide bandgap. Journal of Applied Physics, 2022, 131, . | 2.5 | 24 |
| 32 | A novel two-dimensional sp-sp2-sp3 hybridized carbon nanostructure with a negative in-plane Poisson ratio and high electron mobility. Computational Materials Science, 2020, 185, 109904. | 3.0 | 20 |
| 33 | Six novel carbon and silicon allotropes with their potential application in photovoltaic field. Journal of Physics Condensed Matter, 2020, 32, 355701. | 1.8 | 20 |
| 34 | The Mechanical and Electronic Properties of Carbon-Rich Silicon Carbide. Materials, 2016, 9, 333. | 2.9 | 19 |
| 35 | Metallic and semiconducting carbon allotropes comprising of pentalene skeletons. Diamond and Related Materials, 2020, 109, 108063. | 3.9 | 19 |
| 36 | Mechanical and electronic properties of Ca1â^'Mg O alloys. Materials Science in Semiconductor Processing, 2015, 40, 676-684. | 4.0 | 18 |

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|---|---|---|---|
| 37 | P2<sub>1</sub>3 BN: a novel large-cell boron nitride polymorph. Communications in Theoretical Physics, 2021, 73, 125701. | 2.5 | 18 |
| 38 | Siâ€“Ge alloys in C2/c phase with tunable direct band gaps: A comprehensive study. Current Applied Physics, 2019, 19, 1325-1333. | 2.4 | 17 |
| 39 | Designing a sp3 nanoporous structure of carbon: A comprehensive study on the physical properties. Results in Physics, 2020, 19, 103473. | 4.1 | 17 |
| 40 | Physical properties of Siâ€“Ge alloys in C2/m phase: a comprehensive investigation. Journal of Physics Condensed Matter, 2019, 31, 255703. | 1.8 | 16 |
| 41 | Designing a sp3 structure of carbon T-C9: First-principles calculations. Results in Physics, 2020, 19, 103690. | 4.1 | 16 |
| 42 | Siâ€“C alloys with direct band gaps for photoelectric application. Vacuum, 2022, 199, 110952. | 3.5 | 16 |
| 43 | Two-Dimensional Tetrahex-GeC<sub>2</sub>: A Material with Tunable Electronic and Optical Properties Combined with Ultrahigh Carrier Mobility. ACS Applied Materials & Interfaces, 2021, 13, 14489-14496. | 8.0 | 15 |
| 44 | A Novel Silicon Allotrope in the Monoclinic Phase. Materials, 2017, 10, 441. | 2.9 | 14 |
| 45 | Superhard three-dimensional carbon with one-dimensional conducting channels. New Journal of Chemistry, 2020, 44, 19789-19795. | 2.8 | 14 |
| 46 | Thermodynamic, elastic, elastic anisotropy and minimum thermal conductivity of Î²-GaN under high temperature. Chinese Journal of Physics, 2017, 55, 400-411. | 3.9 | 13 |
| 47 | Mechanical and electronic properties of Si Ge alloy in Cmmm structure. Chinese Journal of Physics, 2016, 54, 298-307. | 3.9 | 12 |
| 48 | Structural, Mechanical, Anisotropic, and Thermal Properties of AlAs in oC12 and hP6 Phases under Pressure. Materials, 2018, 11, 740. | 2.9 | 12 |
| 49 | Direct and quasi-direct band gap silicon allotropes with low energy and strong absorption in the visible for photovoltaic applications. Results in Physics, 2020, 18, 103271. | 4.1 | 12 |
| 50 | Elastic anisotropy and electronic properties of Si3N4 under pressures. AIP Advances, 2016, 6, . | 1.3 | 11 |
| 51 | Novel III-V Nitride Polymorphs in the P42/mnm and Pbca Phases. Materials, 2020, 13, 3743. | 2.9 | 11 |
| 52 | A New Phase of GaN. Journal of Chemistry, 2016, 2016, 1-9. | 1.9 | 10 |
| 53 | Group 14 semiconductor alloys in the P41212 phase: A comprehensive study. Results in Physics, 2021, 25, 104254. | 4.1 | 10 |
| 54 | Theoretical prediction of new Câ€“Si alloys in ${oldsymbol{C}}2/{oldsymbol{m}}$-20 structure. Chinese Physics B, 2017, 26, 046101. | 1.4 | 9 |

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|---|---|---|---|
| 55 | Electronic, Mechanical and Elastic Anisotropy Properties of X-Diamondyne (X = Si, Ge). Materials, 2019, 12, 3589. | 2.9 | 9 |
| 56 | Four Carbon Allotropes Form COT Structures. ACS Applied Electronic Materials, 2022, 4, 2353-2363. | 4.3 | 9 |
| 57 | Mechanical and electronic properties of Câ€“Si alloys in the P222 1 structure. Chinese Journal of Physics, 2016, 54, 700-710. | 3.9 | 8 |
| 58 | Ima2 C32: An orthorhombic carbon allotrope with direct band gap. Diamond and Related Materials, 2021, 120, 108602. | 3.9 | 8 |
| 59 | Low-energy Ga<sub>2</sub>O<sub>3</sub> polymorphs with low electron effective masses. Physical Chemistry Chemical Physics, 2022, 24, 7045-7049. | 2.8 | 8 |
| 60 | Structural, Electronic, and Thermodynamic Properties of Tetragonal t-SixGe3â^'xN4. Materials, 2018, 11, 397. | 2.9 | 7 |
| 61 | Semimetallic 2D Alkynyl Carbon Materials with Distorted Type I Dirac Cones. Journal of Physical Chemistry C, 2021, 125, 18022-18030. | 3.1 | 7 |
| 62 | Effective mass anisotropy of Si-Ge alloys: a discussion of the effective mass tensor. Physica Scripta, 2020, 95, 115808. | 2.5 | 7 |
| 63 | Two novel large-cell boron nitride polymorphs. Diamond and Related Materials, 2022, 126, 109046. | 3.9 | 7 |
| 64 | Direct and quasi-direct band gap of novel Si-Ge alloys in P-3m1 phase. Journal of Physics Condensed Matter, 2021, 33, 385702. | 1.8 | 6 |
| 65 | Tower carbon: a new large-cell carbon allotrope. Journal of Physics Condensed Matter, 2022, 34, 365702. | 1.8 | 5 |
| 66 | 3D superhard metallic carbon network with 1D multi-threaded conduction. Diamond and Related Materials, 2021, 120, 108706. | 3.9 | 4 |
| 67 | Three new C N compounds in orthorhombic symmetry: Theoretical investigations. Diamond and Related Materials, 2022, 127, 109181. | 3.9 | 4 |
| 68 | Three non-metallic carbon materials with comparable electrical conductivity to metals. Diamond and Related Materials, 2022, 128, 109230. | 3.9 | 4 |
| 69 | Structural, Electronic, and Optical Properties of Hexagonal XC 6 (X=N, P, As, and Sb) Monolayers. ChemPhysChem, 2021, 22, 1124-1133. | 2.1 | 0 |