## Qingyang Fan

List of Publications by Year in descending order

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Οινογάνο Γάν

| #  | Article  | IF  | CITATIONS |
|----|--|-----|-----------|
| 1  | Physical properties of group 14 elements in P2/m phase. Journal of Solid State Chemistry, 2022, 305, 122641.   | 2.9 | 24        |
| 2  | All <i>sp</i> 2 hybridization BN polymorphs with wide bandgap. Journal of Applied Physics, 2022, 131, .  | 2.5 | 24        |
| 3  | Si–C alloys with direct band gaps for photoelectric application. Vacuum, 2022, 199, 110952.  | 3.5 | 16        |
| 4  | 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         |
| 5  | Four Carbon Allotropes Form COT Structures. ACS Applied Electronic Materials, 2022, 4, 2353-2363.  | 4.3 | 9         |
| 6  | Two novel large-cell boron nitride polymorphs. Diamond and Related Materials, 2022, 126, 109046.   | 3.9 | 7         |
| 7  | Three new C N compounds in orthorhombic symmetry: Theoretical investigations. Diamond and Related Materials, 2022, 127, 109181.  | 3.9 | 4         |
| 8  | Tower carbon: a new large-cell carbon allotrope. Journal of Physics Condensed Matter, 2022, 34, 365702.  | 1.8 | 5         |
| 9  | Three non-metallic carbon materials with comparable electrical conductivity to metals. Diamond and Related Materials, 2022, 128, 109230.   | 3.9 | 4         |
| 10 | Two-dimensional carbon allotropes with tunable direct band gaps and high carrier mobility. Applied Surface Science, 2021, 537, 147885.   | 6.1 | 39        |
| 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 | Enhanced direct interspecies electron transfer with transition metal oxide accelerants in anaerobic digestion. Bioresource Technology, 2021, 320, 124294.  | 9.6 | 52        |
| 13 | Three-dimensional metallic carbon allotropes with superhardness. Nanotechnology Reviews, 2021, 10, 1266-1276.  | 5.8 | 24        |
| 14 | Two-Dimensional Tetrahex-GeC <sub>2</sub> : A Material with Tunable Electronic and Optical<br>Properties Combined with Ultrahigh Carrier Mobility. ACS Applied Materials & Interfaces, 2021, 13,<br>14489-14496. | 8.0 | 15        |
| 15 | Structural, Electronic, and Optical Properties of Hexagonal XC 6 (X=N, P, As, and Sb) Monolayers.<br>ChemPhysChem, 2021, 22, 1124-1133.  | 2.1 | 0         |
| 16 | Two orthorhombic superhard carbon allotropes: C16 and C24. Diamond and Related Materials, 2021, 116, 108426.   | 3.9 | 35        |
| 17 | Group 14 semiconductor alloys in the P41212 phase: A comprehensive study. Results in Physics, 2021, 25, 104254.  | 4.1 | 10        |
| 18 | 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         |

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|----|---|-----|-----------|
| 19 | P2 <sub>1</sub> 3 BN: a novel large-cell boron nitride polymorph. Communications in Theoretical Physics, 2021, 73, 125701.  | 2.5 | 18        |
| 20 | Semimetallic 2D Alkynyl Carbon Materials with Distorted Type I Dirac Cones. Journal of Physical Chemistry C, 2021, 125, 18022-18030.  | 3.1 | 7         |
| 21 | An orthorhombic superhard carbon allotrope: Pmma C24. Journal of Solid State Chemistry, 2021, 300, 122260.  | 2.9 | 33        |
| 22 | Ima2 C32: An orthorhombic carbon allotrope with direct band gap. Diamond and Related Materials, 2021, 120, 108602.  | 3.9 | 8         |
| 23 | 3D superhard metallic carbon network with 1D multi-threaded conduction. Diamond and Related Materials, 2021, 120, 108706.   | 3.9 | 4         |
| 24 | PBCFâ€Graphene: A 2D <i>Sp</i> <sup>2</sup> Hybridized Honeycomb Carbon Allotrope with a Direct<br>Band Gap. ChemNanoMat, 2020, 6, 139-147.   | 2.8 | 54        |
| 25 | 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        |
| 26 | Superhard three-dimensional carbon with one-dimensional conducting channels. New Journal of Chemistry, 2020, 44, 19789-19795.   | 2.8 | 14        |
| 27 | 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        |
| 28 | Novel III-V Nitride Polymorphs in the P42/mnm and Pbca Phases. Materials, 2020, 13, 3743.   | 2.9 | 11        |
| 29 | Designing a sp3 nanoporous structure of carbon: A comprehensive study on the physical properties.<br>Results in Physics, 2020, 19, 103473.  | 4.1 | 17        |
| 30 | Metallic and semiconducting carbon allotropes comprising of pentalene skeletons. Diamond and<br>Related Materials, 2020, 109, 108063.   | 3.9 | 19        |
| 31 | Physical Properties of XN (X = B, Al, Ga, In) in the Pmâ^'3n phase: First-Principles Calculations. Materials, 2020, 13, 1280.   | 2.9 | 25        |
| 32 | P63/mmc-Ge and their Si–Ge alloys with a mouldable direct band gap. Semiconductor Science and Technology, 2020, 35, 055012.   | 2.0 | 26        |
| 33 | Physical properties of a novel microporous carbon material. Diamond and Related Materials, 2020, 106, 107831.   | 3.9 | 31        |
| 34 | Penta-C20: A Superhard Direct Band Gap Carbon Allotrope Composed of Carbon Pentagon. Materials, 2020, 13, 1926.   | 2.9 | 31        |
| 35 | Six novel carbon and silicon allotropes with their potential application in photovoltaic field. Journal of Physics Condensed Matter, 2020, 32, 355701.                                    | 1.8 | 20        |
| 36 | Five carbon allotropes from Squaroglitter structures. Computational Materials Science, 2020, 178, 109634.   | 3.0 | 49        |

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|----|---|------|-----------|
| 37 | Designing a sp3 structure of carbon T-C9: First-principles calculations. Results in Physics, 2020, 19, 103690.  | 4.1  | 16        |
| 38 | Effective mass anisotropy of Si-Ge alloys: a discussion of the effective mass tensor. Physica Scripta, 2020, 95, 115808.  | 2.5  | 7         |
| 39 | Physical properties of Si–Ge alloys in <i>C</i> 2/ <i>m</i> phase: a comprehensive investigation. Journal of Physics Condensed Matter, 2019, 31, 255703.  | 1.8  | 16        |
| 40 | Physical properties of group 14 semiconductor alloys in orthorhombic phase. Journal of Applied Physics, 2019, 126, 045709.  | 2.5  | 24        |
| 41 | Two novel superhard carbon allotropes with honeycomb structures. Journal of Applied Physics, 2019, 126, .   | 2.5  | 41        |
| 42 | Si–Ge alloys in C2/c phase with tunable direct band gaps: A comprehensive study. Current Applied Physics, 2019, 19, 1325-1333.  | 2.4  | 17        |
| 43 | A hybrid niobium-based oxide with bio-based porous carbon as an efficient electrocatalyst in<br>photovoltaics: a general strategy for understanding the catalytic mechanism. Journal of Materials<br>Chemistry A, 2019, 7, 14864-14875. | 10.3 | 74        |
| 44 | Electronic, Mechanical and Elastic Anisotropy Properties of X-Diamondyne (X = Si, Ge). Materials, 2019, 12, 3589.   | 2.9  | 9         |
| 45 | <i>t</i> ‣i <sub>64</sub> : A Novel Silicon Allotrope. ChemPhysChem, 2019, 20, 128-133.   | 2.1  | 45        |
| 46 | Theoretical investigations of Ge1â^'xSn x alloys (x = 0, 0.333, 0.667, 1) in P42/ncm phase. Journal of<br>Materials Science, 2018, 53, 9611-9626.   | 3.7  | 26        |
| 47 | Theoretical investigations of group IV alloys in the Lonsdaleite phase. Journal of Materials Science, 2018, 53, 2785-2801.  | 3.7  | 31        |
| 48 | Structural, Mechanical, Anisotropic, and Thermal Properties of AlAs in oC12 and hP6 Phases under<br>Pressure. Materials, 2018, 11, 740.   | 2.9  | 12        |
| 49 | Structural, Electronic, and Thermodynamic Properties of Tetragonal t-SixGe3â^'xN4. Materials, 2018, 11, 397.  | 2.9  | 7         |
| 50 | Illâ€Nitride Polymorphs: XN (X=Al, Ga, In) in the <i>Pnma</i> Phase. Chemistry - A European Journal, 2018,<br>24, 17280-17287.  | 3.3  | 46        |
| 51 | Thermodynamic, elastic, elastic anisotropy and minimum thermal conductivity of β-GaN under high<br>temperature. Chinese Journal of Physics, 2017, 55, 400-411.  | 3.9  | 13        |
| 52 | Theoretical prediction of new C–Si alloys in \${oldsymbol{C}}2/{oldsymbol{m}}\$-20 structure.<br>Chinese Physics B, 2017, 26, 046101.   | 1.4  | 9         |
| 53 | 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        |
| 54 | A Novel Silicon Allotrope in the Monoclinic Phase. Materials, 2017, 10, 441.  | 2.9  | 14        |

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|----|--|---|------------------|
| 55 | A New Phase of GaN. Journal of Chemistry, 2016, 2016, 1-9.   | 1.9   | 10               |
| 56 | Si96: A New Silicon Allotrope with Interesting Physical Properties. Materials, 2016, 9, 284.   | 2.9   | 26               |
| 57 | The Mechanical and Electronic Properties of Carbon-Rich Silicon Carbide. Materials, 2016, 9, 333.  | 2.9   | 19               |
| 58 | Two Novel C3N4 Phases: Structural, Mechanical and Electronic Properties. Materials, 2016, 9, 427.  | 2.9   | 34               |
| 59 | Elastic anisotropy and electronic properties of Si3N4 under pressures. AIP Advances, 2016, 6, .  | 1.3   | 11               |
| 60 | 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               |
| 61 | Mechanical and electronic properties of Si Ge alloy in Cmmm structure. Chinese Journal of Physics, 2016, 54, 298-307.  | 3.9   | 12               |
| 62 | Mechanical and electronic properties of C–Si alloys in the P222 1 structure. Chinese Journal of Physics, 2016, 54, 700-710.  | 3.9   | 8                |
| 63 | Two novel silicon phases with direct band gaps. Physical Chemistry Chemical Physics, 2016, 18, 12905-12913.  | 2.8   | 50               |
| 64 | Prediction of novel phase of silicon and Si–Ge alloys. Journal of Solid State Chemistry, 2016, 233,<br>471-483.  | 2.9   | 37               |
| 65 | Novel silicon allotropes: Stability, mechanical, and electronic properties. Journal of Applied Physics, 2015, 118, .   | 2.5   | 44               |
| 66 | Structural, mechanical, and electronic properties of P3m1-BCN. Journal of Physics and Chemistry of Solids, 2015, 79, 89-96.  | 4.0   | 79               |
| 67 | Elastic and electronic properties of Imm2- and I <mmi:math<br>xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif"<br/>overflow="scroll"&gt;<mmi:mrow><mmi:mover<br>accent="true"&gt;<mmi:mrow><mmi:mn>4</mmi:mn></mmi:mrow><mmi:mrow><mmi:mo><td>3.0<br/>1row&gt;<td>25<br/>ml:mover&gt;&lt;</td></td></mmi:mo></mmi:mrow></mmi:mover<br></mmi:mrow></mmi:math<br> | 3.0<br>1row> <td>25<br/>ml:mover&gt;&lt;</td> | 25<br>ml:mover>< |
| 68 | Computational Materials Science, 2015, 97, 6-13.<br>Mechanical and electronic properties of Ca1â^'Mg O alloys. Materials Science in Semiconductor<br>Processing, 2015, 40, 676-684.  | 4.0   | 18               |
| 69 | Elastic and electronic properties of Pbca-BN: First-principles calculations. Computational Materials Science, 2014, 85, 80-87.   | 3.0   | 114              |