Giovanni Pizzi

List of Publications by Year in descending order

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CIOVANNI PIZZI

| # | Article | IF | CITATIONS |
|----|--|------|-----------|
| 1 | An updated version of wannier90: A tool for obtaining maximally-localised Wannier functions. Computer Physics Communications, 2014, 185, 2309-2310. | 3.0 | 1,561 |
| 2 | Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds. Nature Nanotechnology, 2018, 13, 246-252. | 15.6 | 1,317 |
| 3 | Wannier90 as a community code: new features and applications. Journal of Physics Condensed Matter, 2020, 32, 165902. | 0.7 | 807 |
| 4 | Band structure diagram paths based on crystallography. Computational Materials Science, 2017, 128, 140-184. | 1.4 | 457 |
| 5 | AiiDA: automated interactive infrastructure and database for computational science. Computational Materials Science, 2016, 111, 218-230. | 1.4 | 399 |
| 6 | Performance of arsenene and antimonene double-gate MOSFETs from first principles. Nature Communications, 2016, 7, 12585. | 5.8 | 278 |
| 7 | BoltzWann: A code for the evaluation of thermoelectric and electronic transport properties with a maximally-localized Wannier functions basis. Computer Physics Communications, 2014, 185, 422-429. | 3.0 | 219 |
| 8 | Materials Cloud, a platform for open computational science. Scientific Data, 2020, 7, 299. | 2.4 | 189 |
| 9 | AiiDA 1.0, a scalable computational infrastructure for automated reproducible workflows and data provenance. Scientific Data, 2020, 7, 300. | 2.4 | 142 |
| 10 | Radiative recombination and optical gain spectra in biaxially strained <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>n</mml:mi>-type germanium. Physical Review B, 2013, 87, .</mml:math | 1.1 | 64 |
| 11 | Workflows in AiiDA: Engineering a high-throughput, event-based engine for robust and modular computational workflows. Computational Materials Science, 2021, 187, 110086. | 1.4 | 63 |
| 12 | OPTIMADE, an API for exchanging materials data. Scientific Data, 2021, 8, 217. | 2.4 | 49 |
| 13 | Engineering polar discontinuities in honeycomb lattices. Nature Communications, 2014, 5, 5157. | 5.8 | 43 |
| 14 | AiiDAlab – an ecosystem for developing, executing, and sharing scientific workflows. Computational Materials Science, 2021, 188, 110165. | 1.4 | 40 |
| 15 | Automated high-throughput Wannierisation. Npj Computational Materials, 2020, 6, . | 3.5 | 39 |
| 16 | Near- and far-infrared absorption and electronic structure of Ge-SiGe multiple quantum wells. Physical Review B, 2010, 82, . | 1.1 | 37 |
| 17 | Tight-binding calculation of optical gain in tensile strained [001]-Ge/SiGe quantum wells. Nanotechnology, 2010, 21, 055202. | 1.3 | 36 |
| 18 | Conduction band intersubband transitions in Ge/SiGe quantum wells. Applied Physics Letters, 2009, 95, 051918. | 1.5 | 26 |

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|----|---|------|-----------|
| 19 | Long intersubband relaxation times in <i>n</i> -type germanium quantum wells. Applied Physics Letters, 2011, 99, . | 1.5 | 26 |
| 20 | Optical absorption spectra of ultrathin PTCDA films on gold single crystals: Charge transfer beyond the first monolayer. Organic Electronics, 2009, 10, 1448-1453. | 1.4 | 24 |
| 21 | A posteriori metadata from automated provenance tracking: integration of AiiDA and TCOD. Journal of Cheminformatics, 2017, 9, 56. | 2.8 | 24 |
| 22 | Valley-Engineering Mobilities in Two-Dimensional Materials. Nano Letters, 2019, 19, 3723-3729. | 4.5 | 23 |
| 23 | Shear and Breathing Modes of Layered Materials. ACS Nano, 2021, 15, 12509-12534. | 7.3 | 22 |
| 24 | Data Management Plans: the Importance of Data Management in the BIGâ€MAP Project**. Batteries and Supercaps, 2021, 4, 1803-1812. | 2.4 | 19 |
| 25 | Quantum-confined direct-gap transitions in tensile-strained Ge/SiGe multiple quantum wells. Applied Physics Letters, 2011, 99, 031907. | 1.5 | 18 |
| 26 | Workflow Engineering in Materials Design within the BATTERY 2030 + Project. Advanced Energy Materials, 2022, 12, . | 10.2 | 18 |
| 27 | Virtual Computational Chemistry Teaching Laboratories—Hands-On at a Distance. Journal of Chemical Education, 2021, 98, 3163-3171. | 1.1 | 15 |
| 28 | Strain-induced polar discontinuities in two-dimensional materials from combined first-principles and SchrĶdinger-Poisson simulations. Physical Review B, 2017, 96, . | 1.1 | 13 |
| 29 | Microscopic picture of paraelectric perovskites from structural prototypes. Physical Review Research, 2022, 4, . | 1.3 | 11 |
| 30 | Modeling picosecond electron dynamics of pump-probe intersubband spectroscopy in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi mathvariant="bold-italic">n-type Ge/SiGe quantum wells. Physical Review B, 2012, 86, .</mml:mi </mml:math | 1.1 | 10 |
| 31 | An updated version of BoltzWann: A code for the evaluation of thermoelectric and electronic transport properties with a maximally-localized Wannier functions basis. Computer Physics Communications, 2014, 185, 2311-2312. | 3.0 | 10 |
| 32 | Common workflows for computing material properties using different quantum engines. Npj Computational Materials, 2021, 7, . | 3.5 | 10 |
| 33 | Optical gain in short period Si/Ge superlattices on [001]-SiGe substrates. Journal of Applied Physics, 2011, 110, . | 1.1 | 7 |
| 34 | Effect of C-face 4H-SiC(0001) deposition on thermopower of single and multilayer graphene in AA, AB and ABC stacking. 2D Materials, 2014, 1, 035002. | 2.0 | 6 |
| 35 | Provenance, workflows, and crystallographic tools in materials science: AiiDA, spglib, and seekpath. MRS Bulletin, 2018, 43, 696-702. | 1.7 | 6 |
| 36 | Curvature effects on valley splitting and degeneracy lifting: Case of Si/Ge rolled-up nanotubes. Physical Review B, 2012, 85, . | 1.1 | 2 |

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|----|--|-----|-----------|
| 37 | Origins of visible-light emissions in porous silicon. Physica Status Solidi C: Current Topics in Solid State Physics, 2012, 9, 1458-1461. | 0.8 | 2 |
| 38 | Comparison of confinement characters between porous silicon and silicon nanowires. Physics Letters, Section A: General, Atomic and Solid State Physics, 2011, 375, 2422-2429. | 0.9 | 1 |
| 39 | Open-Science Platform for Computational Materials Science: AiiDA and the Materials Cloud. , 2018, , 1-24. | | 1 |
| 40 | Open-Science Platform for Computational Materials Science: AiiDA and the Materials Cloud. , 2020, , 1813-1835. | | 1 |
| 41 | Terahertz intersubband transitions in the conduction band of Ge/SiGe multi quantum wells. , 2010, , . | | 0 |
| 42 | Magnetic field control of intersubband polaritons in narrow-gap semiconductors. Physical Review B, 2011, 83, . | 1.1 | 0 |
| 43 | Terahertz spectroscopy of germanium quantum wells on silicon substrate for terahertz photonics. , 2012, , . | | 0 |
| 44 | Integration of Theoretical Crystallography Open Database and AiiDA. Acta Crystallographica Section A: Foundations and Advances, 2015, 71, s494-s494. | 0.0 | 0 |