

# Publications of Audrius Alkauskas

## Edited books and special issues

1. A. Alkauskas, P. Deák, J. Neugebauer, A. Pasquarello, and C. G. Van de Walle (editors), "*Electronic Structure Methods. Advanced Calculations for Defects in Materials*" (Wiley-VCH, Berlin, 2011).
2. A. Alkauskas, L. C. Bassett, A. Exarhos, and K.-M. Fu (editors), "*Quantum Nanophotonics in Emerging Materials*", special issue of Nanophotonics (DeGruyter, November 2019).

## Articles in scientific journals

Summary: **62 research articles**

**Physical Review Letters** – 4

**Physical Review B** – 22

**Physical Review X** – 2

**Applied Physics Letters** – 6

**Journal of Applied Physics** – 2

**New Journal of Physics** – 1

**Physica Status Solidi** – 4

**Journal of Physical Chemistry** – 3

**Nano Letters** – 2

**ACS Nano / ACS Photonics** – 2

**Nanophotonics** – 2

**Annual Review of Materials Research** – 1

**OSA journals** – 1

other – 10

Web of Science data (2020.05.09): total citations – 2,442; *h*-index – 27, citations per article – 35.9

62. C. E. Dreyer, J. L. Lyons, A. Alkauskas, and C. G. Van de Walle, "*Radiative capture rates at deep defects from electronic structure calculations*", *Phys. Rev. B* **102**, 085305 (2020)
61. D. Wickramaratne, C. E. Dreyer, J.-X. Shen, J. L. Lyons, A. Alkauskas, C. G. Van de Walle, "*Deep-level defects and impurities in InGaN alloys*", *Phys. Status Solidi B* **257**, 1900534 (2020)
60. L. Skuja, K. Smits, A. Trukhin, F. Gahbauer, R. Ferber, M. Auzins, L. Busaite, L. Razinkovas, M. Mackoitis-Sinkevičienė, and A. Alkauskas, "*Dynamics of singlet oxygen molecule trapped in silica glass, studied by luminescence polarization anisotropy and density functional theory*", *J. Phys. Chem. C* **124**, 7244 (2020)
59. M. Mackoitis-Sinkevičienė, M. Maciaszek, C. G. Van de Walle, and A. Alkauskas, "*Carbon dimer defect as the origin of the 4.1 eV luminescence in hexagonal boron nitride*", *Appl. Phys. Lett.* **115**, 212101 (2019)
58. L. C. Bassett, A. Alkauskas, A. L. Exarhos, and K.-M. C. Fu, "*Quantum defects by design*", *Nanophotonics* **8**, 1867 (2019)
57. L. M. Oberg, E. Huang, P. M. Reddy, A. Alkauskas, A. D. Greentree, J. H. Cole, N. B. Manson, C. A. Meriles, and M. W. Doherty, "*Spin coherent quantum transport of electrons between defects in diamond*", *Nanophotonics* **8**, 1975 (2019)

56. M. Turiansky, A. Alkauskas, L. C. Bassett, and C. G. Van de Walle, “*Dangling bonds in hexagonal boron nitride as single-photon emitters*”, Phys. Rev. Lett. **123**, 127401 (2019)
55. Y. K. Frodason, K. M. Johansen, A. Alkauskas, and L. Vines, “*Negative-U and polaronic behavior of the Zn-O divacancy in ZnO*”, Phys. Rev. B **99**, 174106 (2019)
54. D. Wickramaratne, J.-X. Shen, C. E. Dreyer, A. Alkauskas, and C. G. Van de Walle, “*Electrical and optical properties of iron in GaN, AlN, and InN*”, Phys. Rev. B **99**, 205202 (2019)
53. D. Wickramaratne, C. E. Dreyer, B. Monserrat, J.-X. Shen, J. L. Lyons, A. Alkauskas, and C. G. Van de Walle, “*Defect identification based on first-principles calculations for deep level transient spectroscopy*”, Appl. Phys. Lett. **113**, 192106 (2018)
52. N. V. Proscia, Z. Shotton, H. Jayakumar, P. Reddy, M. Dollar, A. Alkauskas, M. W. Doherty, C. A. Meriles, and V. M. Menon, “*Near-deterministic activation of room temperature quantum emitters in hexagonal boron nitride*”, Optica **5**, 1128 (2018)
51. E. Londero, G. Thiering, L. Razinkovas, A. Gali, and A. Alkauskas, “*Vibrational properties of the negatively charged silicon-vacancy complex in diamond from ab initio calculations*”, Phys. Rev. B **98**, 035306 (2018)
50. L. Weston, D. Wickramaratne, M. Mackoite, A. Alkauskas, and C. G. Van de Walle, “*Native point defects and impurities in hexagonal boron nitride*”, Phys. Rev. B **97**, 214104 (2018)
49. Y. K. Frodason, K. M. Johansen, T. S. Bjørheim, B. G. Svensson, and A. Alkauskas, “*Zn vacancy-donor impurity complexes in ZnO*”, Phys. Rev. B **97**, 104109 (2018)
48. C. E. Dreyer, A. Alkauskas, J. L. Lyons, A. Janotti, and C. G. Van de Walle, “*First-principles calculations of defects for quantum technologies*”, Annu. Rev. Mater. Res. **48**, 1 (2018)
47. D. Wickramaratne, J.-X. Shen, A. Alkauskas, and C. G. Van de Walle, “*Comment on “Comparative study of ab initio nonradiative recombination rate calculations under different formalisms”*”, Phys. Rev. B **97**, 077301 (2018)
46. M. Pfender, N. Aslam, P. Simon, D. Antonov, G. Thiering, S. Burk, F. Favaro de Oliveira, A. Denisenko, H. Fedder, J. Meijer, J. A. Garrido, A. Gali, T. Teraji, J. Isoya, M. W. Doherty, A. Alkauskas, A. Gallo, A. Grüneis, P. Neumann, and J. Wrachtrup, “*Protecting a diamond quantum memory by charge state control*”, Nano Letters **17**, 5931 (2017)
45. T. B. Biktagirov, A. N. Smirnov, V. Yu. Davydov, M. W. Doherty, A. Alkauskas, B. C. Gibson, and V. A. Soltamov, “*Strain broadening of the 1042-nm zero-phonon line of the NV center in diamond: a promising spectroscopic tool for defect tomography*”, Phys. Rev. B **96**, 075205 (2017)

44. J. L. Lyons, A. Alkauskas, A. Janotti, and C. G. Van de Walle “*Deep donor state of the copper acceptor as a source of green luminescence in ZnO*”, Appl. Phys. Lett. **111**, 042101 (2017)
43. A. L. Exarhos, D. A. Hopper, R. R. Grote, A. Alkauskas, and L. C. Bassett, “*Optical signatures of quantum emitters in suspended hexagonal boron nitride*”, ACS Nano **11**, 3328 (2017)
42. Y. K. Frodason, K. M. Johansen, T. S. Bjørheim, B. G. Svensson, and A. Alkauskas , “*Zn vacancy as a polaronic hole trap in ZnO*”, Phys. Rev. B **95**, 094105 (2017)
41. J.-X. Shen, D. Wickramaratne, E. Young, C. E. Dreyer, A. Alkauskas, J. S. Speck, and C. G. Van de Walle, “*Calcium as a nonradiative recombination center in InGaN*”, Appl. Phys. Express **10**, 021001 (2017)
40. Z. Shotan, H. Jayakumar, C. R. Conside, M. Mackoit, H. Fedder, J. Wrachtrup, A. Alkauskas, M. W. Doherty, V. Menon, and C. A. Meriles, “*Photo-induced modification of single-photon emitters in hexagonal boron nitride*”, ACS Photonics **3**, 2490 (2016)
39. M. W. Doherty, C. A. Meriles, A. Alkauskas, H. Fedder, M. Sellars, and N. B. Manson, “*Towards a room-temperature spin quantum bus in diamond via electron photoionization, transport and capture*”, Phys. Rev. X **6**, 041035 (2016)
38. D. Wickramaratne, J. Xuan-Shen, C. E. Dreyer, M. Engel, M. Marsman, G. Kresse, S. Marcinkevičius, A. Alkauskas, and C. G. Van de Walle, “*Iron as a source of efficient Shockley-Read-Hall recombination in GaN*”, Appl. Phys. Lett. **109**, 162107 (2016)
37. A. Alkauskas, C. E. Dreyer, J. L. Lyons, and C. G. Van de Walle, “*Role of excited states in Shockley-Read-Hall recombination in wide-band-gap semiconductors*”, Phys. Rev. B **93**, 201304 (2016).
36. A. Alkauskas, M. D. McCluskey, and C. G. Van de Walle, “*Defects in semiconductors – combining experiment and theory*”, J. Appl. Phys. **119**, 181101 (2016)
35. C. E. Dreyer, A. Alkauskas, J. L. Lyons, J. S. Speck, and C. G. Van de Walle, “*Gallium vacancy complexes as a cause of Shockley-Read-Hall recombination in III-nitride light emitters*”, Appl. Phys. Lett. **108**, 141101 (2016)
34. J. L. Lyons, A. Alkauskas, A. Janotti, and C. G. Van de Walle, “*First-principles theory of acceptors in nitride semiconductors*”, Phys. Stat. Solidi B **252**, 900 (2015)
33. B. Himmetoglu, A. Janotti, H. Peelaers, A. Alkauskas, and C. G. Van de Walle, “*First-principles study of the mobility of SrTiO<sub>3</sub>*”, Phys. Rev. B **90**, 241204 (2014)
32. A. Alkauskas, Q. Yan, and C. G. Van de Walle, “*First-principles theory of nonradiative capture via multiphonon emission*”, Phys. Rev. B **90**, 075202 (2014)
31. A. Alkauskas, B. B. Buckley, D. D. Awschalom, and C. G. Van de Walle, “*First-principles theory of the luminescence lineshape for the triplet transition in diamond NV centres*”, New J. Phys. **16**, 073023 (2014)

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23. A. Alkauskas, P. Broqvist, and A. Pasquarello, “*Energy levels of defects from hybrid functionals: insights and applications*”, Phys. Stat. Solidi B **248**, 775 (2011)
22. A. Alkauskas, S. Schneider, S. Sagmeister, C. Ambrosch-Draxl, and C. Hébert, “*Theoretical analysis of the momentum-dependent loss function of bulk Ag*”, Ultramicroscopy **110**, 1081 (2010)
21. P. Broqvist, A. Alkauskas, and A. Pasquarello, “*A hybrid functional scheme for the determination of defect levels and band alignment at semiconductor-oxide interfaces*”, Phys. Stat. Solidi A **207**, 270 (2010)
20. A. Carvalho, A. Alkauskas, A. Pasquarello, A. Tagantsev, and N. Setter, “*Li-related defects in ZnO: hybrid functional calculations*”, Physica B **404**, 4797 (2009)
19. A. Carvalho, A. Alkauskas, A. Pasquarello, A. Tagantsev, and N. Setter, “*A hybrid density functional study of lithium in ZnO: Stability, ionization levels, and diffusion*”, Phys. Rev. B **80**, 195205 (2009)
18. P. Broqvist, A. Alkauskas, and A. Pasquarello, “*Hybrid-functional calculations with plane-wave basis sets: The effect of the singularity correction on total energies, energy eigenvalues, and defect energy levels*”, Phys. Rev. B **80**, 085114 (2009)

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13. P. Broqvist, A. Alkauskas, and A. Pasquarello, “*Defect levels of dangling bonds in silicon and germanium through hybrid functionals*”, Phys. Rev. B **78**, 075203 (2008)
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