Publications of Audrius Alkauskas

Books

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).

Articles in scientific journals

Summary: **50 research articles**

Physical Review Letters – 3	**Nano Letters** – 2
Physical Review X – 2	**ACS Nano** / **ACS Photonics** – 2
Physical Review B – 18	**Journal of Physical Chemistry** – 2
Applied Physics Letters – 4	**Annual Reviews** – 1
Journal of Applied Physics – 2	**Physica Status Solidi** – 3
New Journal of Physics – 1	other – 10

Web of Science data: total citations – 1610, *h*-index – 21, citations per article – 30.3

52. E. Londero, G. Thiering, A. Gali, and A. Alkauskas, "*Vibrational properties of the negatively charged silicon-vacancy complex in diamond from ab initio calculations*", submitted to Phys. Rev. B (2018).

51. N. V. Proscia, Z. Shoton, 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*", submitted to Optica (2018).

50. L. Weston, D. Wickramaratne, M. Mackoit, A. Alkauskas, and C. G. Van de Walle, "*Native point defects and impurities in hexagonal boron nitride*", Phys. Rev. B **97**, XXXXXX (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., in press (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. Considine, 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 SrTiO3*", 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)

30. A. Alkauskas, S. D. Schneider, S. Sagmeister, C. Hébert, and C. Draxl, "*Dynamic structure factors of Cu, Ag, and Au: Comparative study from first principles*", Phys. Rev. B **88**, 195124 (2013)

29. A. Alkauskas, J. L. Lyons, D. Steiauf, and C. G. Van de Walle, "*First-Principles calculations of luminescence spectrum line shapes for defects in semiconductors: the example of GaN and ZnO*", Phys. Rev. Lett. **109**, 267401 (2012)

28. D. M. Toyli, D. J. Christle, A. Alkauskas, B. Buckley, C. G. Van de Walle, and D. D. Awschalom, "*Measurement and control of single nitrogen-vacancy center spins above 600 K*", Phys. Rev. X **2**, 031001 (2012)

27. F. Devynck, A. Alkauskas, P. Broqvist, and A. Pasquarello, "*Charge transition levels of carbon-, oxygen-, and hydrogen-related defects at the SiC/SiO2 interface through hybrid functionals*", Phys. Rev. B **84**, 235320 (2011)

26. A. Alkauskas and A. Pasquarello, "*Bang-edge problem in theoretical determination of defect energy levels: The O vacancy in ZnO as a benchmark case*", Phys. Rev. B **84**, 125206 (2011)

25. C. Hébert, A. Alkauskas, S. Löffler, B. Jouffrey, and P. Schattschneider, "*Capturing EELS in the reciprocal space*", Eur. Phys. J. Appl. Phys. **54**, 33510 (2011)

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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)

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17. P. Broqvist, A. Alkauskas, J. Godet, and A. Pasquarello, "*First principles investigation of defect energy levels at semiconductor-oxide interfaces: O vacancies and H interstitials at Si-SiO2-HfO2 stacks*", J. Appl. Phys. **105**, 061603 (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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3. A. Alkauskas, B. Y. K. Hu, K. Flensberg, and A. P. Jauho, "*Sign reversal of drag in bilayer systems with in-plane periodic potential modulation*", Phys. Rev. B **66**, 201304 (2002)

2. A. Alkauskas, "*Tunneling of edge states. Non-interacting electrons*", Lith. J. Phys. **42**, 17 (2002)

1. A. Alkauskas, J. Čeponkus, V. Aleksa, B. Mikulskienė, E. Butkus, and V. Šablinskas, "*Conformational stability of bicyclo[3.3.1]nonane-2,6-dione and bicyclo[3.3.1]nonane-2,9-dione studied by vibrational spectroscopy and ab initio calculations*", J. Mol. Struct. **563**, 517 (2001)