

# Timothy B. Boykin

## DEGREES

Ph.D. (Electrical Engineering), Stanford University, 1992.

*A Tight-Binding Approach to Resonant Tunneling Diode Simulation*, 1992.

Prof. James S. Harris, Jr., advisor.

M.S. (Electrical Engineering), Stanford University, 1988.

B.S.E.E., *summa cum laude*, Rice University, 1987.

## EMPLOYMENT and EXPERIENCE

*September, 1992 - Present*

Department of Electrical and Computer Engineering, The University of Alabama in Huntsville.

Professor (August, 2007-Present).

Associate Professor (August, 1997-August, 2007; tenured since August, 2008).

Assistant Professor (September, 1992-August, 1997).

*June, 1992 - September, 1992*

Post-Doctoral Research Associate, Department of Electrical Engineering, Stanford University.

*June, 1988 - June, 1992*

Research Assistant, Department of Electrical Engineering, Stanford University.

*Summers, 1984 - 1987*

MITRE Corporation, Houston, Texas. Computer system performance evaluation.

## HONORS and AWARDS

*Fellow*, Institute of Electrical and Electronics Engineers, 2018.

*Fellow*, American Physical Society, 2011.

ACM Gordon Bell Prize, Honorable Mention (SC11), 2011.

UAH College of Engineering Outstanding Faculty Award, 2012.

UAH Foundation Research Award (Applied Research), 2001.

Elected to Sigma Xi, 1994.

Stanford Graduate Fellowship, 1987-88.

Elected to Phi Beta Kappa, 1987.

Elected to Tau Beta Pi, 1986.

Elected to Eta Kappa Nu, 1986.

## PROFESSIONAL SOCIETIES

American Physical Society, Fellow.

IEEE, Fellow.

Referee/Reviewer for: *Physical Review Letters*, *Physical Review B*, *Physical Review E*, *Journal of Physics: Condensed Matter*, *New Journal of Physics*, *American Journal of Physics*, *European Journal of Physics*, *IEEE Transactions on Electron Devices*, *IEEE Electron Device Letters*, *IEEE Transactions on Nanotechnology*, *Journal of Applied Physics*, *Applied Physics Letters*, *Journal of Computational Electronics*, *Solid State Communications*, *Physica B & E*.

## BOOK CHAPTERS/ENCYCLOPEDIA ARTICLES

5. S. Ahmed, N. Kharche, R. Rahman, M. Usman, S. Lee, H. Ryu, H. Bae, S. Clark, B. Haley, M. Naumov, F. Saied, M. Korkusinski, R. Kennel, M. McLennan, T. Boykin, and G. Klimeck, "Multimillion Atom Simulation of Electronic and Optical Properties of Nanoscale Devices using NEMO 3-D," in *Encyclopedia of Complexity and System Science*, 1-69, (Springer, New York, 2015). (Updated edition from 2009 & 2013.) [UAH]
4. S. Ahmed, N. Kharche, R. Rahman, M. Usman, S. Lee, H. Ryu, H. Bae, S. Clark, B. Haley, M. Naumov, F. Saied, M. Korkusinski, R. Kennel, M. McLennan, T. Boykin, and G. Klimeck, "Multimillion Atom Simulation of Electronic and Optical Properties of Nanoscale Devices using NEMO 3-D," in *Encyclopedia of Complexity and System Science*, Article ID: 60515, Chapter ID: 343, (Springer, New York, 2013). [UAH]
3. S. Ahmed, N. Kharche, R. Rahman, M. Usman, S. Lee, H. Ryu, H. Bae, S. Clark, B. Haley, M. Naumov, F. Saied, M. Korkusinski, R. Kennel, M. McLennan, T. Boykin, and G. Klimeck, "Multimillion Atom Simulations with NEMO 3-D," in *Encyclopedia of Complexity and System Science*, vol. 6, ed. R. A. Meyers, pp. 5745-5783, (Springer, New York, 2009). [UAH]
2. Timothy B. Boykin, "Quantum Mechanical Description of Solids," sec. 6.4.3.3 of *Encyclopedia of Life Support Systems (EOLSS)*, UNESCO-sponsored (2001) [UAH].
1. Timothy B. Boykin, "Tailoring Empirical Tight-Binding Models for Semiconductor Heterostructures," in Stoyan J. Vlaev and L. M. Gaggero-Sager, eds., *Some Contemporary Problems of Condensed Matter Physics*, (Nova Science Publishers, Huntington, New York, 2000), pp. 39-63. [UAH]

## REFEREED JOURNAL ARTICLES

The code in square brackets following each entry indicates the institution at which the work was performed: University of Alabama in Huntsville [UAH] or Stanford University [SU].

*Published or Accepted for Publication*

96. Sijay Huang, Timothy B. Boykin, Ravi S. Gorur, and Biswajit Ray, "Electrical Tree Formation in Polymer-Filler Composites," *IEEE Transactions on Dielectrics and Electrical Insulation* (in press). [UAH]
95. Timothy B. Boykin, "The discretized momentum operator," *The Physics Educator* **1**, 1920003 (2019). [UAH]
94. Timothy B. Boykin, Prasad Sarangapani, and Gerhard Klimeck, "Non-orthogonal tight-binding models: Problems and possible remedies for realistic nano-scale devices," *Journal of Applied Physics* **125**, 144302 (2019). [UAH]
93. M. Raquibuzzaman, B. Ray, T. B. Boykin, and R. S. Gorur, "Polymer-Metal Layered Structures for Improved Energy Storage Density," *IEEE Transactions on Dielectrics and*

*Electrical Insulation* **25**, 2375 (2018). [UAH]

92. Timothy B. Boykin and Arvind Ajoy, “Effective bandstructures from unfolding supercells with vacancies,” *Physica B* **531**, 130 (2018). [UAH]
91. Timothy B. Boykin and Gerhard Klimeck, “Insights from simple models for surface states in nanostructures,” *European Journal of Physics* **38**, 025501 (2017). [UAH]
90. Yaohua Tan, Michael Povolotskyi, Tillmann Kubis, Timothy B. Boykin, and Gerhard Klimeck, “Transferable tight-binding model for strained group IV and III-V materials and heterostructures,” *Physical Review B* **94**, 045311 (2016). [UAH]
89. Timothy B. Boykin, Arvind Ajoy, Hesameddin Ilatikhameneh, Michael Povolotskyi, and Gerhard Klimeck, “Unfolding and effective bandstructure calculations as discrete real- and reciprocal-space operations,” *Physica B* **491**, 22 (2016). [UAH]
88. Yaohua P. Tan, Michael Povolotskyi, Tillmann Kubis, Timothy B. Boykin, and Gerhard Klimeck, “Tight-binding analysis of Si and GaAs ultrathin bodies with subatomic wavefunction resolution,” *Physical Review B* **92**, 085301 (2015). [UAH]
87. Timothy B. Boykin, Arvind Ajoy, Hesameddin Ilatikhameneh, Michael Povolotskyi, and Gerhard Klimeck, “Brillouin zone unfolding method for effective phonon spectra,” *Physical Review B* **90**, 205214 (2014). [UAH]
86. SungGeun Kim, Mathieu Luisier, Timothy B. Boykin, and Gerhard Klimeck, “Computational Study of Heterojunction Graphene Nanoribbon Tunneling Transistors with p/d Orbital Tight-binding Method,” *Applied Physics Letters* **104**, 243113 (2014). [UAH]
85. Ganesh Hegde, Michael Povolotskyi, Tillmann Kubis, Timothy Boykin, and Gerhard Klimeck, “An environment-dependent semi-empirical tight binding model suitable for electron transport in bulk metals, metal alloys, metallic interfaces, and metallic nanostructures. I. Model and validation,” *Journal of Applied Physics* **115**, 123703 (2014). [UAH]
84. Timothy B. Boykin, “Effective interactions and block diagonalization in quantum-mechanical problems,” *Journal of Mathematical Chemistry* **52**, 1599 (2014). [UAH]
83. Neerav Kharche, Timothy B. Boykin, and Saroj K. Nayak, “Multiscale Modeling of Screening Effects on Conductivity of Graphene in Weakly Bonded Graphene-Dielectric Heterostructures,” *Journal of Computational Electronics* **12**, 722 (2013). [UAH]
82. Xueping Jiang, Neerav Kharche, Paul Kohl, Timothy B. Boykin, Gerhard Klimeck, Mathieu Luisier, Pulickel M. Ajayan, and Saroj K. Nayak, “Giant Quasiparticle Band Gap Modulation in Graphene Nanoribbons Supported on Weakly Interacting Surfaces,” *Applied Physics Letters* **103**, 133107 (2013). [UAH]

81. M. Luisier, T. B. Boykin, Z. Ye, A. Martini, G. Klimeck, N. Kharche, X. Jaing, and S. Nayak, "Investigation of ripple-limited low-field mobility in large-scale graphene nanoribbons," *Applied Physics Letters* **102**, 253506 (2013). [UAH]
80. Zhengping Jiang, Marcelo A. Kuroda, Yaohua Tan, Dennis M. Newns, Michael Povolotskyi, Timothy B. Boykin, Tillmann Kubis, Gerhard Klimeck, and Glenn J. Martyna, "Electron transport in nano-scaled piezoelectronic devices," *Applied Physics Letters* **102**, 193501 (2013). [UAH]
79. Yaohua Tan, Michael Povolotskyi, Tillmann Kubis, Yu He, Zhengping Jiang, Gerhard Klimeck, and Timothy B. Boykin, "Empirical tight-binding parameters for GaAs and MgO with explicit basis through DFT mapping," *Journal of Computational Electronics* **12**, 56 (2013). [UAH]
78. Mehdi Salmani-Jelodar, Abhijeet Paul, Timothy Boykin, and Gerhard Klimeck, "Calculation of phonon spectrum and thermal properties in suspended  $\langle 100 \rangle$   $\text{In}_x\text{Ga}_{1-x}\text{As}$  nanowires," *Journal of Computational Electronics* **11**, 22 (2012) (INVITED). [UAH]
77. Zhengping Jiang, Neerav Kharche, Timothy Boykin, and Gerhard Klimeck, "Effects of interface disorder on valley splitting in SiGe/Si/SiGe quantum wells," *Applied Physics Letters* **100**, 103502 (2012). [UAH]
76. Sung Geun Kim, Mathieu Luisier, Timothy B. Boykin, and Gerhard Klimeck, "Effects of interface roughness scattering on radio frequency performance of silicon nanowire transistors," *Applied Physics Letters* **99**, 232107 (2011). [UAH]
75. Muhammad Usman, Yui-Hong Matthias Tan, Hoon Ryu, Shaikh S. Ahmed, Hubert J. Krenner, Timothy B. Boykin, and Gerhard Klimeck, "Quantitative excited state spectroscopy of a single InGaAs quantum dot molecule through multi-million-atom electronic structure calculations," *Nanotechnology* **22**, 315709 (2011). [UAH]
74. Timothy B. Boykin, Mathieu Luisier, Gerhard Klimeck, Xueping Jiang, Neerav Kharche, and Saroj K. Nayak, "Accurate six-band nearest-neighbor tight-binding model for the  $\pi$ -bands of bulk graphene and graphene nanoribbons," *Journal of Applied Physics* **109**, 104304 (2011) [UAH].
73. SungGeun Kim, Abhijeet Paul, Mathieu Luisier, Timothy B. Boykin, and Gerhard Klimeck, "Full Three-Dimensional Quantum Transport Simulation of Atomistic Interface Roughness in Silicon Nanowire FETs," *IEEE Transactions on Electron Devices* **58**, 1371 (2011). [UAH]
72. Timothy B. Boykin, Mathieu Luisier, and Gerhard Klimeck, "Current density and continuity in discretized models," *European Journal of Physics* **31**, 1077 (2010); Corrigendum **32**, 631 (2011). [UAH]

71. Timothy B. Boykin, Mathieu Luisier, Mehdi Salmani-Jelodar, and Gerhard Klimeck, "Strain-induced, off-diagonal, same-atom parameters in empirical tight-binding theory suitable for [110] uniaxial strain applied to a silicon parameterization," *Physical Review B* **81**, 125202 (2010). [UAH]
70. Samarth Agarwal, Kyle H. Montgomery, Timothy B. Boykin, Gerhard Klimeck, and Jerry M. Woodall, "Design Guidelines for True Green LEDs and High Efficiency Photovoltaics Using ZnSe/GaAs Digital Alloys," *Electrochemical and Solid State Letters* **13**, H5 (2010). [UAH]
69. Timothy B. Boykin, "Recent developments in tight-binding approaches for nanowires," *Journal of Computational Electronics* **8**, 142 (2009). (INVITED) [UAH]
68. Rajib Rahman, Seung H. Park, Timothy B. Boykin, Gerhard Klimeck, Sven Rogge, and Lloyd C. L. Hollenberg, "Gate-induced g-factor control and dimensional transition for donors in multivalley semiconductors," *Physical Review B* **80**, 115301 (2009). [UAH]
67. Neerav Kharche, Seongmin Kim, Timothy B. Boykin, and Gerhard Klimeck, "Valley degeneracies in (111) silicon quantum wells," *Applied Physics Letters* **94**, 042101 (2009). [UAH]
66. Timothy B. Boykin, Neerav Kharche, and Gerhard Klimeck, "Non-primitive rectangular supercells for tight-binding electronic structure calculations," *Physica E* **41**, 490 (2009). [UAH]
65. Neerav Kharche, Mathieu Luisier, Timothy B. Boykin, and Gerhrd Klimeck, "Electronic structure and transmission characteristics of SiGe Nanowires," *Journal of Computational Electronics* **7**, 350 (2008). [UAH]
64. Timothy B. Boykin, Neerav Kharche, and Gerhard Klimeck, "Valley splitting in finite barrier quantum wells," *Physical Review B* **77**, 245320 (2008). [UAH]
63. Timothy B. Boykin, Mathieu Luisier, and Gerhard Klimeck, "Multi-band transmission calculations for nanowires using an optimized renormalization method," *Physical Review B* **77**, 165318 (2008). [UAH]
62. Timothy B. Boykin, Neerav Kharche, and Gerhard Klimeck, "Brillouin zone unfolding of perfect supercells having non-equivalent primitive cells illustrated with a Si/Ge tight-binding parameterization," *Physical Review B* **76**, 035310 (2007). [UAH]
61. Gerhard Klimeck, Shaikh Ahmed, Neerav Kharche, Marek Korkusinski, Muhammad Usman, Marta Prada, and Timothy B. Boykin, "Atomistic simulation of realistically sized nanodevices using NEMO 3-D: II-Applications," *IEEE Transactions on Electron Devices* **54**, 2090 (2007). [UAH]
60. Gerhard Klimeck, Shaikh Ahmed, Neerav Kharche, Marek Korkusinski, Muhammad Usman,

- Marta Prada, and Timothy B. Boykin, "Atomistic simulation of realistically sized nanodevices using NEMO 3-D: I-Models and Benchmarks," *IEEE Transactions on Electron Devices* **54**, 2079 (2007). [UAH]
59. Timothy B. Boykin, Neerav Kharche, and Gerhard Klimeck, "Evolution time and energy uncertainty," *European Journal of Physics* **28**, 673 (2007). [UAH]
  58. Neerav Kharche, Marta Prada, Timothy B. Boykin, and Gerhard Klimeck, "Valley-splitting in strained silicon quantum wells modeled with 2° miscuts, step disorder, and alloy disorder," *Applied Physics Letters* **90**, 092109 (2007). [UAH]
  57. Timothy B. Boykin, Neerav Kharche, Gerhard Klimeck, and Marek Korkusinski, "Approximate bandstructures of semiconductor alloys from tight-binding supercell calculations," *Journal of Physics: Condensed Matter* **19**, 036203 (2007). [UAH]
  56. Timothy B. Boykin, Mathieu Luisier, Andreas Schenk, Neerav Kharche, and Gerhard Klimeck, "The electronic structure and transmission characteristics of disordered AlGaAs nanowires," *IEEE Transactions on Nanotechnology* **6**, 43 (2007). [UAH]
  55. Timothy B. Boykin, Neerav Kharche, and Gerhard Klimeck, "Allowed wavevectors under the application of incommensurate periodic boundary conditions," *European Journal of Physics* **27**, 5 (2006). [UAH]
  54. A. S. Martins, Timothy B. Boykin, Gerhard Klimeck, and Belita Koiller, "Conduction-band tight-binding description for Si applied to P donors," *Physical Review B* **72**, 193204 (2005). [UAH]
  53. Timothy B. Boykin and Gerhard Klimeck, "The discretized Schrödinger equation for the finite square well and its relationship to solid state physics," *European Journal of Physics* **26**, 865 (2005). [UAH]
  52. Dennis Hite, Timothy B. Boykin, Nagendra Singh, and Dashen Shen, "A simple Fermi-Dirac Integrating Circuit," *American Journal of Physics* **73**, 856 (2005). [UAH]
  51. Anisur Rahman, Gerhard Klimeck, Mark Lundstrom, Nizami Vagidov, and Timothy B. Boykin, "Atomistic Approach for Nano-Scale Devices at the Scaling Limit and Beyond - Valley Splitting in Si", *Japanese Journal of Applied Physics* **44**, 2187 (2005). [UAH]
  50. Yun Zheng, Cristian Rivas, Roger Lake, Khairul Alam, Timothy B. Boykin, and Gerhard Klimeck, "Electronic Properties of Silicon Nanowires", *IEEE Transactions on Electron Devices* **52**, 1097 (2005). [UAH]
  49. Jeremy Green, Timothy B. Boykin, Corrie D. Farmer, Michel Garcia, Charles N. Ironside, Gerhard Klimeck, Roger Lake, and Colin R. Stanley, "Quantum cascade laser gain medium modeling using a second-nearest-neighbor  $sp^3s^*$  tight-binding model", *Superlattices and*

*Microstructures* **37**, 410 (2005). [UAH]

48. Timothy B. Boykin, Gerhard Klimeck, Paul von Allmen, Fabiano Oyafuso, and Seungwon Lee, "Valley splitting in V-shaped quantum wells," *Journal of Applied Physics* **97**, 113702 (2005). [UAH]
47. Timothy B. Boykin and Gerhard Klimeck, "Practical application of zone-folding concepts in tight-binding," *Physical Review B* **71**, 115215 (2005). [UAH]
46. Timothy B. Boykin, Gerhard Klimeck, Mark Friesen, S. N. Coppersmith, Paul von Allmen, Fabiano Oyafuso, and Seungwon Lee, "Valley-splitting in low-density quantum-confined heterostructures studied using tight-binding models," *Physical Review B* **70**, 165325 (2004). [UAH]
45. Timothy B. Boykin and Gerhard Klimeck, "The discretized Schrödinger equation and simple models for semiconductor quantum wells," *European Journal of Physics* **25**, 503 (2004). [UAH]
44. Timothy B. Boykin, Gerhard Klimeck, and Fabiano Oyafuso, "Valence band effective mass expressions in the  $sp^3d^5s^*$  empirical tight-binding model applied to a Si and Ge parameterization," *Physical Review B* **69**, 115201 (2004). [UAH]
43. Timothy B. Boykin, Gerhard Klimeck, Mark Eriksson, Mark Friesen, S. N. Coppersmith, Paul von Allmen, Fabiano Oyafuso, and Seungwon Lee, "Valley splitting in strained Si quantum wells," *Applied Physics Letters* **84**, 115 (2004). [UAH]
42. Fabiano Oyafuso, Gerhard Klimeck, Paul von Allmen, Timothy B. Boykin, and R. Chris Bowen, "Strain effects in large-scale atomistic quantum dot simulations," *Physica Status Solidi b* **239**, 71 (2003). [UAH]
41. Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, Timothy B. Boykin, and Paul von Allmen, "Disorder-induced broadening in multimillion atom alloyed quantum dot systems," *Physica Status Solidi c* **0004**, 1149 (2003). [UAH]
40. Timothy B. Boykin, "Derivatives of the Dirac delta function by explicit construction of sequences," *American Journal of Physics* **71**, 462 (2003). [UAH]
39. Timothy B. Boykin, Gerhard Klimeck, R. Chris Bowen, and Fabiano Oyafuso, "Diagonal parameter shifts due to nearest-neighbor displacements in empirical tight-binding theory," *Physical Review B* **66**, 125207 (2002). [UAH]
38. Gerhard Klimeck, Fabiano Oyafuso, Timothy B. Boykin, R. Chris Bowen, and Paul von Allmen, "Development of a Nanoelectronic 3-D (NEMO 3-D) Simulator for Multimillion Atom Simulations and Its Application to Alloyed Quantum Dots," *Journal of Computer Modeling in Engineering and Science* **3**, 601 (2002); invited. [UAH]

37. Gerhard Klimeck, Fabiano Oyafuso, R. Chris Bowen, Timothy B. Boykin, Thomas A. Cwik, Edith Huang, and Edward Vinyard, "3-D Atomistic Nanoelectronic Modeling on High Performance Clusters: Multimillion Atom Simulations", *Superlattices and Microstructures* **31**, 171 (2002). [UAH]
36. Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Atomistic Electronic Structure Calculations of Unstrained Alloyed Systems Consisting of a Million Atoms", *Journal of Computational Electronics* **1**, 317 (2002). [UAH]
35. Timothy B. Boykin, Dennis Hite, and Nagendra Singh, "The two-capacitor problem with radiation," *American Journal of Physics* **70**, 415 (2002). [UAH]
34. Timothy B. Boykin and P. Vogl, "Dielectric response of molecules in empirical tight-binding theory," *Physical Review B* **65** 035202 (2001). [UAH]
33. Timothy B. Boykin, R. Chris Bowen, and Gerhard Klimeck, "Electromagnetic coupling and gauge invariance in the empirical tight-binding method," *Physical Review B* **63**, 245314 (2001). [UAH]
32. Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Off zone-center or indirect bandgap-like hole transport in heterostructures," *Physical Review B* **63**, 195310 (2001). [UAH]
31. Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Strong wavevector dependence of hole transport in heterostructures," *Superlattices and Microstructures* **29**, 187 (2001). [UAH]
30. Timothy B. Boykin, "Tight-binding-like expressions for the continuous-space electromagnetic coupling Hamiltonian." *American Journal of Physics* **69**, 793 (2001). [UAH]
29. Gerhard Klimeck, R. Chris Bowen, Timothy B. Boykin, and Thomas A. Cwik, " $sp^3s^*$  tight-binding parameters for transport simulations in compound semiconductors," *Superlattices and Microstructures* **27**, 519 (2000). [UAH]
28. Gerhard Klimeck, R. Chris Bowen, Timothy B. Boykin, Carlos Salazar-Lazaro, Thomas A. Cwik, and Adrian Stoica, "Tight-binding models for Si quantum devices and parameter fitting using genetic algorithms," *Superlattices and Microstructures* **27**, 77 (2000). [UAH]
27. Timothy B. Boykin, "An alternative view of the continuity equation in quantum mechanics," *American Journal of Physics* **68**, 665 (2000). [UAH]
26. Timothy B. Boykin, "Exact representation of  $\exp(i\mathbf{q}\mathbf{r})$  in the empirical tight-binding method and its application to electromagnetic interactions," *Physical Review B* **60**, 15 810 (1999). [UAH]



25. Timothy B. Boykin, R. Chris Bowen, Gerhard Klimeck, and Kevin L. Lear, “Resonant-tunneling diodes with emitter prewells,” *Applied Physics Letters* **75**, 1302 (1999). [UAH]
24. J.G. Menchero and Timothy B. Boykin, “Impurity states in semiconductors calculated via tight-binding: a parameter sensitivity study,” *Physical Review B* **59**, 8137 (1999). [UAH]
23. Timothy B. Boykin, Roger K. Lake, Gerhard Klimeck, and Mukund Swaminathan, “Interface effects in tunneling models with identical real and complex dispersions,” *Physical Review B* **59**, 7316 (1999). [UAH]
22. Timothy B. Boykin, Lisa J. Gamble, Gerhard Klimeck, and R. Chris Bowen, “Valence-band warping in tight-binding models,” *Physical Review B* **59**, 7301 (1999). [UAH]
21. Timothy B. Boykin, “A more physical formulation of the self-inductance for spatially distributed circuits,” *American Journal of Physics* **67**, 320 (1999). [UAH]
20. Timothy B. Boykin, “More complete treatment of spin-orbit effects in tight-binding models,” *Physical Review B* **57**, 1620 (1998). [UAH]
19. Timothy B. Boykin, “Improved fits of effective masses at  $\Gamma$  in the spin-orbit, second-nearest-neighbor  $sp^3s^*$  model: results from analytic expressions,” *Physical Review B* **56**, 9613 (1997). [UAH]
18. Timothy B. Boykin, Gerhard Klimeck, R. Chris Bowen, and Roger Lake, “Effective mass reproducibility of the nearest-neighbor  $sp^3s^*$  models: analytic results,” *Physical Review B* **56**, 4102 (1997); Erratum **61**, 5033 (2000). [UAH]
17. Timothy B. Boykin and Herman C. Chui, “Simplified treatment of many-body effects in the intersubband absorption of symmetric, uniformly doped quantum wells at zero temperature,” *Physical Review B* **55**, 7091 (1997). [UAH]
16. Timothy B. Boykin, “Tunneling calculations for systems with singular coupling matrices: results for a simple model,” *Physical Review B* **54**, 7670 (1996). [UAH]
15. Timothy B. Boykin, “Generalized eigenproblem method for surface and interface states: the complex bands of GaAs and AlAs,” *Physical Review B* **54**, 8107 (1996). [UAH]
14. Timothy B. Boykin, “Incorporation of incompleteness in the  $\mathbf{kp}$  perturbation theory,” *Physical Review B* **52**, 16 317 (1995). [UAH]
13. Timothy B. Boykin and C.D. Johnson, “A generalized solution expression for linear, homogeneous, constant-coefficient difference equations,” *Journal of the Franklin Institute* **332B**, 227 (1995). [UAH]
12. Timothy B. Boykin, “Approximations for the resonant-tunneling diode current: implications

for triple-barrier devices,” *Journal of Applied Physics* **78**, 6818 (1995). [UAH]

11. Timothy B. Boykin, “Current-voltage calculations for InAs/AlSb resonant-tunneling diodes,” *Physical Review B* **51**, 4289 (1995). [UAH]
10. Timothy B. Boykin, R.E. Carnahan, and K.P. Martin, “Inadequacy of the one-dimensional approximation for resonant-tunneling diode current-voltage calculations,” *Physical Review B* **51**, 2273 (1995). [UAH]
9. Timothy B. Boykin, R.E. Carnahan, and K.P. Martin, “Validity of the semiclassical interpretation of resonant magnetotunneling experiments,” *Physical Review B* **50**, 15 393 (1994). [UAH]
8. Timothy B. Boykin, “Conduction-band states of thin InAs/AlSb quantum wells,” *Applied Physics Letters* **64**, 1529 (1994). [UAH]
7. Timothy B. Boykin, R.E. Carnahan, and R.J. Higgins, “Quantum well states of InAs/AlSb resonant tunneling diodes,” *Physical Review B* **48**, 14 232 (1993). [UAH]
6. Timothy B. Boykin, “Resonance features of a two-state model,” *Physical Review B* **47**, 12696 (1993). [UAH]
5. Timothy B. Boykin, Bardia Pezeshki, and James S. Harris, Jr., “Anti-resonances in the transmission of a simple two-state model,” *Physical Review B* **46**, 12 769 (1992). [SU]
4. Timothy B. Boykin, and James S. Harris, Jr., “X-valley tunneling in single AlAs barriers,” *Journal of Applied Physics* **72**, 988 (1992). [SU]
3. B. Pezeshki, S.M. Lord, T.B. Boykin, and J.S. Harris, Jr., “GaAs/AlAs quantum wells for electroabsorption modulators,” *Applied Physics Letters* **60**, 2779 (1992). [SU]
2. B. Pezeshki, S.M. Lord, T.B. Boykin, B.L. Shoop, and J.S. Harris, Jr., “AlGaAs/GaAs QW modulator for 6328 Å operation,” *Electronics Letters* **27**, 1971 (1991). [SU]
1. Timothy B. Boykin, Jan P.A. van der Wagt, and James S. Harris, Jr., “Tight-binding model for GaAs/AlAs resonant tunneling diodes,” *Physical Review B* **43**, 4777 (1991). [SU]

## CONFERENCE PRESENTATIONS

69. Yaohua Tan, Michael Povolotskyi, Tillmann Kubis, Timothy Boykin, Gerhard Klimeck, “Transferable tight binding model for strained group IV and III-V heterostructures,” APS March Meeting, March 14–18, 2016, Baltimore, Maryland. [UAH]

68. Yaohua Tan, Michael Povolotskyi, Tillmann Kubis, Timothy Boykin, Gerhard Klimeck, "Transferable tight binding model for strained group IV and III-V heterostructure," International Workshop on Computational Electronics (IWCE), West Lafayette, USA, 2015. [UAH]
67. Yaohua Tan, Michael Povolotskyi, Tillmann Kubis, Timothy Boykin, Gerhard Klimeck, "Tight Binding analysis of Si/GaAs UTBs with subatomic resolution," 17th International Workshop on Computational Electronics (IWCE), Paris, France, 2014. [UAH]
66. Zhengping Jiang, Marcelo Kuroda, Yaohua Tan, Dennis News, Glenn Martyna, Michael Povolotskyi, Timothy Boykin, Tillmann Kubis, Gerhard Klimeck, "Tight-Binding Modeling of Intermediate Valence Compound SmSe for Piezoelectronic Devices," 16th International Workshop on Computational Electronics (IWCE), June 2013, Nara, Japan. [UAH]
65. Xueping Jiang, Neerav Kharche, Paul Kohl, Timothy Boykin, Gerhard Klimeck, Mathieu Luisier, Pulickel Ajayan, Saroj Nayak, "Quasiparticle Band Gap modulation in Graphene Nanoribbons Supported on Weakly interacting Surfaces," APS March Meeting, Baltimore, 18-22 Mar 2013. [UAH]
64. SungGeun Kim, Mathieu Luisier, Timothy Boykin, J. Geng, Jim Fonseca, Gerhard Klimeck, "Atomistic Simulation of Graphene Transistors," MSD review May 2012, Boston. [UAH]
63. T. B. Boykin, M. Luisier, N. Kharche, X. Jiang, S. K. Nyak, A. Martini, and G. Klimeck, "Multiband Tight-Binding Model for Strained and Bilayer Graphene from DFT Calculations," 15<sup>th</sup> International Workshop on Computational Electronics (IWCE), University of Wisconsin-Madison, 22-25 May 2012. [UAH]
62. Yaohua P. Tan, Michael Povolotskyi, Tillmann Kubis, Timothy B. Boykin, and Gerhard Klimeck, "Generation of Empirical Tight Binding Parameters from ab-initio Simulations," 15<sup>th</sup> International Workshop on Computational Electronics (IWCE), University of Wisconsin-Madison, 22-25 May 2012. [UAH]
61. Timothy Boykin , Mathieu Luisier , Gerhard Klimeck , Xueping Jiang , Neerav Kharche , Yu Zhou , Saroj Nayak, "Six-band nearest-neighbor tight-binding model for the  $\pi$ -bands of bulk graphene and graphene nanoribbons," APS March 2012 Meeting, Boston, MA. [UAH]
60. Mehdi Salmani-Jelodar, Abhijeet Paul, Timothy Boykin, Gerhard Klimeck, "Phonon Spectrum and Thermal Properties of free standing <100> and <111> InGaAs alloy nanowires," APS March Meeting 2012, Boston, US. [UAH]
59. SungGeun Kim, Mathieu Luisier, Abhijeet Paul, Timothy B. Boykin, Gerhard Klimeck, "Full 3D Quantum Transport Simulation of Atomistic Interface Roughness in Silicon Nanowire FETs," TECHCON 2011. [UAH]
58. Hoon Ryu, Sunhee Lee, Zhengping Jiang, Yui Hong Tan, Michael Povolotskyi, Neerav

Kharche, Mark Eriksson, Timothy Boykin, Gerhard Klimeck, B.Weber, M.Fuechsle, J.Miwa, S.Mahapatra, W.H.Lim, H.Yang, N.Lai, F.Mohiyaddin, A.Morello, A.Dzurak, M.Y.Simmons,L.C.L.Hollenberg, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates," NSA / IARPA / ARO Quantum Computing Technology Workshop, Denver, August 11-12, 2011. [UAH]

57. S. Kim, S. R. Mehrotra, M. Luisier, T. B. Boykin, and G. Klimeck, "Effects of interface roughness scattering on RF performance of nanowire transistors," *2011 International Semiconductor Device Research Symposium (ISDRS)*, 7-9 December 2011. [UAH]
56. M. Luisier, T. B. Boykin, G. Klimeck, and W. Fichtner, "Atomistic nanoelectronic device engineering with sustained performances up to 1.44 PFlops/s," *2011 International Conference for High Performance Computing, Networking, Storage, and Analysis*, 12-18 November 2011. [UAH]
55. Timothy B. Boykin, Zhengping Jiang, Neerav Kharche, and Gerhard Klimeck, "Effect of disorder on the valley-splitting in Si/SiGe quantum wells," Invited, 7th International Workshop on Silicon Quantum Electronics, Denver, CO, 14-15 August 2011. [UAH]
54. M. Rodwell, W. Frensley, S. Steiger, E. Chagarov, S. Lee, H. Ryu. Y. Tan, G. Hegde, L. Wang, J. Law, T. Boykin, G. Klimeck, P. Ashbeck, and A. Kummel, "III-V FET Channel Denigns for High Current Densities and Thin Inversion Layers," *Device Research Conference 2010 (DRC 2010) Digest*, 149 (2010). [UAH]
53. Gerhard Klimeck, Mathieu Luisier, Tim Boykin, Xueping Jiang, Neerav Kharche, Yu Zhou, Saroj K Nayak, "Atomistic Graphene Transistors - New Device or New Material?" *University of Minnessota Nanotech Conference*, Oct 7 and 8, 2010. [UAH]
52. Gerhard Klimeck, Mathieu Luisier, Tim Boykin, Xueping Jiang, Neerav Kharche, Yu Zhou, Saroj K. Nayak, "Atomistic Graphene Transistors - New Device or New Material ?" *NRI Workshop on Carbon Based Electronics*, Albany NY, Sept. 21-22, 2010. [UAH]
51. Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier, Timothy B. Boykin, Gerhard Klimeck, "Strain Engineering of Trigated Silicon Nanowire FinFETs for Improved Device Performance," *TECHCON*, Austin, Texas, Sept. 13-14, 2010. [UAH]
50. Timothy B. Boykin, Neerav Kharche, Muhammed Usman, Rajib Rahman, Gerhard Klimeck, and Mathieu Luisier, "Physics and Numerics of Multi-Band Tight-Binding Nanostructure Model," *CECAM Workshop on Empirical methods in semiconductor nano-structures design and modeling*, ACAM Dublin, Ireland and University of Manchester, Manchester, U.K., June 21-25, 2010. [UAH]
49. Rodwell, M. J. W.; Singiseti, U.; Wistey, M.; Burek, G. J.; Carter, A.; Baraskar, A. ; Law, J.; Thibeault, B. J.; Kim, Eun Ji; Shin, B.; Lee, Yong-ju; Steiger, S.; Lee, S. ; Ryu, H.; Tan, Y.; Hegde, G.; Wang, L.; Chagarov, E.; Gossard, A. C.; Frensley, W.; Kummel, A. ; Palmstrom,

C.; McIntyre, Paul C; Boykin, T.; Klimek, G.; Asbeck, P.; “III-V MOSFETs: Scaling laws, scaling limits, fabrication processes,” 2010 International Conference on Indium Phosphide and Related Materials (IPRM), Takamatsu, Japan, 31 May - 4 June, 2010. [UAH]

48. SungGeun Kim, Abhijeet Paul, Mathieu Luisier, Gerhard Klimeck, and Timothy Boykin, “Full 3D Quantum Transport Simulation of Interface Roughness in Nanowire FETs,” American Physical Society March Meeting 2010. [UAH]
47. Hoon Ryu, Gerhard Klimeck, Sunhee Lee, Rajib Rahman, B Haley, S.H Park, Neerav Kharche, Z Jiang, Timothy B. Boykin, Cameron Wellard, Jared Cole, Lloyd Hollenberg, Gabri Lansbergen, Sven Rogge, Bent Weber, M Simmons, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", International Symposium on Advanced Nanodevices and Nanotechnology (ISANN), Kaanapali, Maui, Nov. 29-Dec. 4, 2009.
46. Hoon Ryu, Gerhard Klimeck, Sunhee Lee, Rajib Rahman, B Haley, S.H Park, Neerav Kharche, Z Jiang, Timothy B. Boykin, Cameron Wellard, Jared Cole, Lloyd Hollenberg, Gabri Lansbergen, Sven Rogge, Bent Weber, M Simmons, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", *Silicon Qubit Workshop*, Univeristy of California Berkeley, Aug. 24-25, 2009.
45. Mathieu Luisier, Andreas Schenk, Wolfgang Fichtner, Timothy B. Boykin, and Gerhard Klimeck, "A parallel sparse linear solver for nearest-neighbor tight-binding problems", 14th International Conference on Parallel and Distributed Computing. August 26-29, 2008 Las Palmas de Gran Canaria, Spain, (2008). [89 accepted papers out of 264 submissions].
44. Timothy B. Boykin, Neerav Kharche, Mathieu Luisier, Gerhard Klimeck, “Zone Unfolding and Approximate Bandstructure Calculations in Tight-Binding”, American Physical Society, March Meeting 2008. [UAH]
43. Neerav Kharche, Seongmin Kim, Timothy B. Boykin, Gerhard Klimeck, “Substrate orientation dependence of valley-splitting in Silicon nanostructures”, American Physical Society, March Meeting 2008. [UAH]
42. Neerav Kharche, Mathieu Luisier, Timothy B. Boykin, and Gerhard Klimeck, "Electronic Structure and Transmission Characteristics of SiGe Nanowires", *The 12th International Workshop on Computational Electronics*, University of Massachusetts Amherst, Oct. 7-10, 2007. [UAH]
41. Neerav Kharche, Marta Prada, Timothy B. Boykin, Gerhard Klimeck, “Valley-splitting in strained Silicon quantum wells on a miscut substrate using tight-binding model”, American Physical Society, March Meeting 2007. [UAH]
40. Gerhard Klimeck, Timothy B. Boykin, Mathieu Luisier, Neerav Kharche, Andreas Schenk,

"Electronic structure and transport in random alloy AlGaAs nanowires", Advanced Heterostructure Workshop, Hawaii, Dec. 3 - 8, 2006. [UAH]

39. Gerhard Klimeck, Timothy Boykin, Mathieu Luisier, Neerav Kharche, Andreas Schenk, "A Study of alloyed nanowires from two perspectives: approximate dispersion diagrams and transmission coefficients", 28th International Conference on the Physics of Semiconductors, ICPS 2006, Vienna, Austria, July 24-28 2006. [UAH]
38. Neerav Kharche, Clemens Heitzinger, Gerhard Klimeck, Mathieu Luisier, Timothy Boykin, "Bandstructure Effects in Unstructured AlGaAs Nanowires", March Meeting of the American Physical Society, Baltimore, MD, March 13-17, (2006). [UAH]
37. Timothy B. Boykin, Gerhard Klimeck, S. N. Coppersmith, Mark Friesen, Paul von Allmen, Seungwon Lee, and Fabiano Oyafuso, "Valley splitting in low-density quantum-confined heterostructures: Superposition, not Spin!", APS March Meeting, Los Angeles, CA, March 21-25, (2005). [UAH]
36. Anisur Rahman, Gerhard Klimeck, Nizami Vagidov, Timothy B. Boykin, and Mark S. Lundstrom, "Nanoscale Device Simulation at the Scaling Limit and Beyond", International Conference on Solid State Devices and Materials (SSDM 2004), Tokyo, Japan, Sept. 14-17, (2004). [UAH]
35. Yun Zheng, Cristian Rivas, Roger Lake, Khairul Alam, Timothy B. Boykin, and Gerhard Klimeck, "Electronic Properties of Silicon Nanowires", IEEE proceedings of the 10th International Workshop for Computational Electronics (IWCE), Purdue University, West Lafayette, Oct. 24-27, (2004). [UAH]
34. Seungwon Lee, Paul von Allmen, Fabiano Oyafuso, Gerhard Klimeck, Timothy B. Boykin, S.N. Coppersmith, Mark Friesen, and Mark Erikson., "Electron Exchange Interaction in Electronically Confined Si Quantum Dots", IEEE proceedings of the 10th International Workshop for Computational Electronics (IWCE), Purdue University, West Lafayette, Oct. 24-27, (2004). [UAH]
33. Gerhard Klimeck, Paul von Allmen, Seungwon Lee, Fabiano Oyafuso, Olga Lazarenkova, Timothy B. Boykin, "Nanoelectronic Modeling (NEMO) for Realistic Simulations of Solid-State Quantum Computing Gates", DARPA Focused Quantum Systems (FoQuS) Workshop, Falls Church, VA, Jan 28-29 (2004). [UAH]
32. Gerhard Klimeck, T. B. Boykin, M. Eriksson, M. Friesen, S. N. Coppersmith, P. von Allmen, F. Oyafuso, S. Lee, "Conduction band valley splitting in Si", March Meeting of the American Physical Society, March 22-26, Montreal, CA (2004). [UAH]
31. Timothy B. Boykin, Gerhard Klimeck, Fabiano Oyafuso, and Paul von Allmen, "Atomistic Quantum Device Simulation in the Si, Ge, and SiGe Material Systems with Realistic

- Bandstructure," Presented at the Second International Workshop on Quantum Dots for Quantum Computing, Notre Dame, IN, August 6-9 (2003). [UAH]
30. Fabiano Oyafuso, Gerhard Klimeck, Timothy B. Boykin, R. Chris Bowen, and Paul von Allmen, "Study of Strain Boundary Conditions and GaAs Buffer Sizes in InGaAs Quantum Dots", International Workshop on Computational Electronics, Frascati, Rome, Italy, May 25-28, 2003. [UAH]
  29. Timothy B. Boykin, Gerhard Klimeck, R. Chris Bowen, and Fabiano Oyafuso, "Diagonal parameter shifts in strained semiconductors in the empirical tight-binding theory", March Meeting of American Physical Society, March 16-21, Austin, TX (2003). [UAH]
  28. Fabiano Oyafuso, Gerhard Klimeck, Timothy B. Boykin\*, R. Chris Bowen, and Paul von Allmen, "Effects of Electronic and Strain Boundary Conditions in Multi-million Atom Electronic Structure Simulations", March Meeting of American Physical Society, March 16-21, Austin, TX (2003). [UAH]
  27. Gerhard Klimeck, Fabiano Oyafuso, R. Chris Bowen, Timothy B. Boykin, and Paul von Allmen, "NEMO 3-D: Multi-Million Atom Electronic Structure Calculation, Simulation of Alloy Disorder in Quantum Dots", The NASA University Research, Engineering, and Technology Institute for Nanoelectronics and Computing (INAC) and The NSF Network for Computational Nanotechnology (NCN), Official Kickoffs and Workshop, Purdue University, West Lafayette, IN, January 15-17, (2003). [UAH]
  26. Gerhard Klimeck, Fabiano Oyafuso, Chris Bowen, Paul von Allmen, Tom Cwik, Ed Vinyard, Edith Huang, Timothy Boykin, "Quantum Dot Modeling using NEMO 3-D: IT Challenges in the development of quantum device simulator", JPL representation in the NASA booth of Supercomputing 2002, Baltimore, MD, Nov 17-22, 2002. [UAH]
  25. Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, Tim Boykin, Paul von Allmen, "Study of Alloy Induced Disorder in Quantum Dots using Tight-binding", 4th Motorola Workshop on Computational Materials and Electronics, Tempe, AZ, Nov 14-15, 2002. [UAH]
  24. Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, Tim Boykin, Paul von Allmen, "Modeling of Disordered Multimillion Atom Quantum Dot Systems", 2nd JPL IT Symposium, Pasadena, CA, Nov 4, 2002. [UAH]
  23. Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, Timothy B. Boykin, and Paul von Allmen, "Boundary Conditions in Disordered Multimillion Atom Quantum Dot Systems", 2nd International Conference on Semiconductor Quantum Dots -QD2002-, September 30 - October 3, 2002 Komaba Campus, University of Tokyo. [UAH]
  22. Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Nanoelectronic 3-D (NEMO 3-D) Simulation of Multimillion Atom Quantum Dot Systems", SISPAD 2002, Kobe, Japan, Sept. 3-6, 2002. [UAH]

21. Gerhard Klimeck, Fabiano Oyafuso, Timothy B. Boykin, and R. Chris Bowen, "Quantum Dot Simulation", AFRL-JPL workshop on Nanotechnology, Pasadena, CA, May 8-10, 2002. [UAH]
20. Gerhard Klimeck, Fabiano Oyafuso, Timothy B. Boykin, and R. Chris Bowen, "Multi-million Atom Electronic Structure Simulations using NEMO 3-D", March Meeting of American Physical Society, March 17-22, Indianapolis, IN (2002). [UAH]
19. Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Atomistic Electronic Structure Calculations of Unstrained Alloyed Systems Consisting of a Million Atoms", *8th International Workshop on Computational Electronics*, October 15-18, 2001, Univ. of Illinois. [UAH]
18. Gerhard Klimeck, Fabiano Oyafuso, R. Chris Bowen, R. Chris Bowen, Timothy B. Boykin, Thomas A. Cwik, Edith Huang, Edward Vinyard, "Quantum Dot Modeling using NEMO 3-D, or Development of a Bottom-Up Nanoelectronic Simulator", Sackler Colloquium, National Academy of Sciences, Washington DC, May 18-20 (2001). [UAH]
17. Gerhard Klimeck, R. Chris Bowen, Timothy B. Boykin, and Fabiano Oyafuso, "Atomistic Quantum Dot Simulation using NEMO-3D", Nanospace 2001, Galveston, Texas, March 13-16 (2001). [UAH]
16. Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Quantum Dot Modeling Using NEMO-3D", given at *March Meeting of the American Physical Society*, Seattle, WA, March 12-16, 2001. [UAH].
15. Timothy B. Boykin, Gerhard Klimeck, and R. Chris Bowen, "A Tiger by the Tail: the Momentum Operator in Tight-Binding", given at *March Meeting of the American Physical Society*, Seattle, WA, March 12-16, 2001. [UAH].
14. Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Transverse Momentum Dependence of Electron and Hole Tunneling in a Full Band Tight-Binding Simulation", *Proceedings of the 27th Symposium on Compound Semiconductors (ISCS)*, IEEE (2000). [UAH]
13. Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Atomistic Simulation of Quantum Dots Including Strain and Bandstructure", given at *Electronic Materials Conference*, Denver, CO, June 21-23, 2000. [UAH]
12. Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Atomistic Simulation of Quantum Dots Including Strain and Bandstructure and Full Band Simulation of Hole Transport in 1-D Heterostructures", given at *International Workshop on Computational Electronics*, Glasgow, UK, May 22-25, 2000. [UAH]
11. Gerhard Klimeck, R. Chris Bowen, Timothy B. Boykin, and Tom Cwik, " $sp^3s^*$  and  $sp^3d^5s^*$



Tight-Binding Parameter Sets for GaAs, AlAs, InAs, GaSb, AlSb, InSb, GaP, AlP, and InP for quantum dot simulations", given at *March Meeting of the American Physical Society*, Minneapolis, MN, March 20-24, 2000. [UAH].

10. Gerhard Klimeck, R. Chris Bowen, Tom Cwik, and Timothy B. Boykin, "A Prototype of a 3-D Nanoelectronic Modeling Tool (NEMO-3D)", given at *Nanospace 2000*, Houston, TX Jan. 23-28, 2000. [UAH]
9. Timothy B. Boykin, Gerhard Klimeck, and R. Chris Bowen, "Nanoelectronic Device Calculation from an atomistic point of view: Empirical Tight-Binding Models for Semiconductor Heterostructures", given at *Nanospace 2000*, Houston, TX Jan. 23-28, 2000. [UAH]
8. Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Development of a 3-D Nanoelectronic Modeling Tool (NEMO-3D)," given at *Surfaces and Interfaces in Mesoscopic Devices*, Maui, HI, 5-10 December, 1999. [UAH]
7. Timothy B. Boykin, Lisa J. Gamble, Gerhard Klimeck, and R. Chris Bowen, "Valence-band warping in tight-binding models and its effect on heterostructure electronic states," given at the *1999 Centennial March Meeting of the American Physical Society*, Atlanta, GA, 20-26 March, 1999. [UAH]
6. Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Tight-binding  $sp^3s^*$  parameters from genetic algorithms," given at the *1999 Centennial March Meeting of the American Physical Society*, Atlanta, GA, 20-26 March, 1999. [UAH]
5. Timothy B. Boykin, Gerhard Klimeck, Roger Lake, and R. Chris Bowen, "The well-tempered tight-binding model: many parameters do not necessarily imply flexibility," given at the *1998 March Meeting of the American Physical Society*, Los Angeles, CA, 16-20 March, 1998. [UAH]
4. Gerhard Klimeck, Daniel K. Blanks, Roger Lake, Timothy B. Boykin, and R. Chris Bowen, "NEMO: a 1-D heterostructure design tool," given at the *1998 March Meeting of the American Physical Society*, Los Angeles, CA, 16-20 March, 1998. [UAH]
3. Jan P.A. van der Wagt, A.C. Seabaugh, G. Klimeck, E.A. Beam III, T.B. Boykin, R.C. Bowen, and R. Lake, "Ultralow current density RTDs for tunneling-based SRAM," given at the *1997 International Symposium on Compound Semiconductors*, San Diego, CA, 7 September 1997. [UAH]
2. Gerhard Klimeck, R. Chris Bowen, Roger Lake, Dan Blanks, Ted Moise, Yung-Chung Kao, Timothy B. Boykin, and William R. Frensley, "Quantitative simulation of strained and unstrained InP-based resonant tunneling diodes," given at the *1997 Device Research Conference*, Fort Collins, CO, 23-25 June 1997. [UAH]
1. Timothy B. Boykin, R.E. Carnahan, and K.P. Martin, "Transmission and current-voltage

characteristics of conduction-band resonant-tunneling diodes: some surprises,” given at the *1995 March Meeting of the American Physical Society*, San Jose, CA, 20-24 March, 1995. [UAH]

## PATENTS

2. T. Brooks Boykin and Timothy B. Boykin,”Programmable hot water heater control method,” U.S. Patent No. 5 103 078 (1992).
1. T. Brooks Boykin and Timothy B. Boykin,”Programmable hot water heater control device,” U.S. Patent No. 5 023 432 (1991).

## SPONSORED RESEARCH

7. Timothy B. Boykin (Principal Investigator), “Empirical tight-binding materials models for revolutionary CMOS devices,” Purdue University (subcontract from SRC contract on which G. Klimeck is PI and T. B. Boykin is a CI), 1 January 2006 - 31 December 2008, UAH part: approx. **\$30 000/year**; additional **\$32 000** for Fall 2006; additional **\$32 000** for Fall 2007; additional **\$32 000** for Fall 2008.
6. Timothy B. Boykin (Principal Investigator), “Tight-binding calculations for strained supercells,” JPL, 1 January 2005 - 31 August 2005, **\$26 781**.
5. Gerhard Klimeck (Principal Investigator, JPL) and Fabiano Oyafuso (Co-Investigator, JPL), and Timothy B. Boykin (Co-Investigator, UAH), “Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates,” NSA, 15 May 2002 - 14 May 2004, **\$75 000/year** (UAH, approx.), \$300 000/year (total JPL and UAH, approx.).
4. Timothy B. Boykin (Principal Investigator), “Models for Quantum-Dot Computing Devices,” JPL, 1 July 2000 - 31 December 2000, **\$80 000** (approx.).
3. Gregory P. Nordin (Principal Investigator), Mustafa Abushagur, Timothy B. Boykin, William E. Cohen, Richard L. Fork, Rhonda K. Gaede, Jeffrey H. Kulick, Dashen Shen, and B. Earl Wells (Co-Investigators), “Integrated research environment for intermeshed optoelectronics,” NSF/EPSCoR, 1 February 1998 - 31 January 2001, \$3 000 000 (approx.).
2. Timothy B. Boykin (Principal Investigator), Renewal of “Tight-binding models for quantum device simulations,” Texas Instruments, Inc., 15 August 1996 - 31 December 1997, **\$24 000** (approx.).
1. Timothy B. Boykin (Principal Investigator), “Tight-binding models for quantum device simulations,” Texas Instruments, Inc., 1 May 1995 - 15 August 1996, **\$40 000** (approx.).

**GRADUATE STUDENTS**

Dennis Hite, MS, Thesis: *A Simple Fermi-Dirac Integrating Circuit*, May 2005.