

ALEX ZUNGER
CHRONOLOGICAL PUBLICATIONS LIST

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1972 (1-2)

1. A. Zunger and K. Bar-Eli, "Non-Linear Behavior of Solutions Illuminated by a Ruby Laser," *J. Chem. Physics* **57**, 3558-3567 (1972).
2. A. Zunger, "Iterative Extended Huckel Calculation on Hexagonal Boron Nitride," *Solid State Commun.* **11**, 1727-1730 (1972).

1974 (3-6)

3. A. Zunger and K. Bar-Eli, "Non-Linear Behavior of Solutions Illuminated by a Ruby Laser II," *IEEE J. of Quantum Electronics QE-10*, 29-36 (1974).
4. A. Zunger, "A Molecular Calculation of Electronic Properties of Layered Crystals. I. Truncated Crystal Approach for Hexagonal Boron-Nitride," *J. Phys. C* **7**, 76-96 (1974).
5. A. Zunger, "A Molecular Calculation of Electronic Properties of Layered Crystals. II Periodic Small Cluster Calculation for Graphite and Boron Nitride," *J. Phys. C* **7**, 96-106 (1974).
6. A. Zunger, "Semiempirical LCAO Calculations on Electronic and Dynamic Properties of α and γ Nitrogen Crystals and Nitrogen Aggregates," *Molecular Physics* **28**, 713-727 (1974).

1975 (7-16)

7. A. Katzir, J. T. Suss, A. Zunger, and A. Halperin, "Point Defects in Hexagonal Boron-Nitride. I. EPR, Thermoluminescence and Thermally-Stimulated-Current Measurements," *Phys. Rev. B* **11**, 2370-2377 (1975).
8. A. Zunger and A. Katzir, "Point Defects in Hexagonal Boron-Nitride. II. Theoretical Studies," *Phys. Rev. B* **11**, 2378-2390 (1975).
9. A. Zunger, "LCAO Truncated Crystal Calculations on Some Electronic Properties of Compressed Molecular Hydrogen Crystals," *J. Phys. Chem. Solids* **36**, 229-238 (1975).
10. A. Zunger, "Small Periodic Cluster Calculations of Perfect and Defect Solids," *Annales de la Societe de Bruxelles T* **89**, 77-97 (1975).
11. A. Zunger and E. Huler, "Calculation of Structural Properties and Vibrational Frequencies in α and γ -N₂ Crystals," *J. Chem. Phys.* **62**, 3010-3023 (1975).
12. A. Zunger, "Small Periodic Cluster Calculation on Point Defect Problems in Hexagonal Layered Solids," *J. Chem. Phys.* **62**, 1861-1868 (1975).
13. A. Zunger, "Band Structure of the One-Dimensional Metallic (SN)_x Crystal," *J. Chem. Phys.* **63**, 4854-4860 (1975).

14. A. Zunger, "Band Structure, Crystal Conformation and Hydrogen Bond Potentials for Solid HF," *J. Chem. Phys.* **63**, 1713-1731 (1975).
15. E. Huler and A. Zunger, "Lattice Dynamics of Solids α and γ Nitrogen Crystals at Various Pressures," *Phys. Rev. B.* **12**, 5878-5889 (1975).
16. E. Huler and A. Zunger, "Calculation of the Equilibrium Configuration and Intermolecular Frequencies of Water Dimers and Hexagonal Ice," *Chem. Phys.* **13**, 433-440 (1975).

1976 (17-19)

17. A. Zunger, A. Katzir, and A. Halperin, "Optical Properties of Hexagonal Boron Nitride," *Phys. Rev. B.* **13**, 5560-5573 (1976).
18. A. Zunger and A. J. Freeman, "Combined Fourier Transform and Discrete Variational Approach to the Self-consistent Solution of the Electronic Band Structure Problem within the Local Density Formalism," *Int. J. of Quantum Chem., Symp.* **10**, 383-403 (1976).
19. A. Zunger and A. J. Freeman, "Self-consistent LCAO Local Density Determination of Anisotropic Compton Profile and X-Ray Structure Factors in Diamond," *Physics Letters* **57A**, 453-457 (1976).

1977 (20-26)

20. A. Zunger and A. J. Freeman, "Self-consistent Numerical Basis Set LCAO Model for the Study of Electronic Properties of Solids in the Local Density Formalism," *Phys. Rev. B.* **15**, 4716-4737 (1977).
21. A. Zunger and A. J. Freeman, "Ground State Electronic Properties of Diamond in the Local Density Formalism," *Phys. Rev. B.* **15**, 5049-5065 (1977).
22. A. Zunger and A. J. Freeman, "Defect State Models for Localized Excitations in LiF," *Physics Letters* **60A**, 456 (1977).
23. A. Zunger and A. J. Freeman, "Self-consistent Numerical Basis Set LCAO Investigation of Electronic and Structural Properties of TiS₂," *Phys. Rev. B.* **16**, 906-924 (1977).
24. A. Zunger and A. J. Freeman, "Ground and Excited State Electronic Properties of LiF in the Local Density Model," *Phys. Rev. B.* **16**, 2901-2926 (1977).
25. S. Topiol, A. Zunger and M. Ratner, "Local Density Pseudopotentials for the First Row Atoms," *Chem. Phys. Lett.* **49**, 367-373 (1977).
26. A. Zunger and A. J. Freeman, "Local Density Formalism Approach to Cohesive Properties of

Diamond, Boron Nitride and Lithium Fluoride," *Int. J. of Quant. Chem.* **S11**, 539-546 (1977).

1978 (27-36)

27. A. Zunger, "Self-consistent LCAO Calculation of the Electronic Properties of Graphite. I. The Regular Graphite Lattice," *Physical Rev. B*. **17**, 625-641, (1978).
28. A. Zunger and R. Englman, "Self-consistent LCAO Calculation of the Electronic Properties of Graphite. II. Point Vacancy in the Two-Dimensional Crystal," *Phys. Rev. B*. **17**, 642-661, (1978).
29. A. Zunger and A. J. Freeman, "Ab Initio Self-Consistent Study of the Electronic Structure and Properties of Cubic Boron Nitride," *Phys. Rev. B*. **17**, 2030-2041 (1978).
30. A. Zunger, "First Principles Theoretical Study on the Electronic Properties of the B32 Intermetallic Compound - LiAl," *Phys. Rev. B*. **17**, 2582-2594 (1978).
31. A. Zunger and A. J. Freeman, "Band Structure and Lattice Instability of TiSe₂," *Phys. Rev. B*. **17**, 1839-1842 (1978).
32. A. Zunger and M. A. Ratner, "On the First Principles Hartree-Fock and Local Density Pseudopotentials," *Chem. Phys.* **30**, 423-443 (1978).
33. A. Zunger and A. J. Freeman, "Electronic Structure and Properties of Cubic CdS," *Phys. Rev. B*. **17**, 4850 (1978).
34. A. Zunger and A. J. Freeman, "Structurally-Induced Semimetal to Semiconductor Transition in TiSe₂," *Physical Review Letters* **40**, 1155 (1978).
35. A. Zunger and M. L. Cohen, "A Density Functional Pseudopotential Approach to Crystal Phase Stability and Electronic Structure," *Physical Review Letters* **41**, 53-56 (1978).
36. A. Zunger and M. L. Cohen, "A First Principles Non-Local Pseudopotential Approach to the Density Functional Formalism. I. Development and Applications to Atoms," *Phys. Rev. B*. **18**, 5449-5472 (1978).

1979 (37-46)

37. A. Zunger, S. Topiol, and M. Ratner, "First Principles Pseudopotentials Model in the Local Density Formalism," *Chem. Phys.* **39**, 75-90 (1979).
38. A. Zunger and A. J. Freeman, "Electronic Structure of lT-VSe₂," *Phys. Rev. B*. **19**, 6001-6009 (1979).
39. A. Zunger and M. L. Cohen, "A First Principles Non-Local Pseudopotential Approach in the

Density Functional Formalism. II. Applications to Electronic and Structural Properties of Solids," *Phys. Rev. B* **20**, 4082-4108 (1979).

40. J. Ihm, A. Zunger, and M. L. Cohen, "A Momentum Space Formalism for the Total Energy of Solids Using Pseudopotentials," *J. Phys. C* **12**, 4409-4421 (1979).
41. A. Zunger and M. L. Cohen, "A Self-Consistent Pseudopotential Calculation of Bulk Properties of Mo and W," *Phys. Rev. B* **19**, 568-582 (1979).
42. A. Zunger, G. P. Kerker, and M. L. Cohen, "Calculation of the Electronic Structure of Molybdenum in a First Principles Non-Local Pseudopotential Approach," *Phys. Rev. B* **20**, 581-593 (1979).
43. G. P. Kerker, A. Zunger, M. L. Cohen, and M. Schluter, "A Solid State Approach to the Electronic Structure of Molecules: A Self-Consistent First-Principles Pseudopotential Calculation for O₂," *Solid State Commun.* **32**, 309-312 (1979).
44. A. Zunger and M. L. Cohen, "Electronic Structure of CuCl," *Phys. Rev. B* **20**, 1189-1193 (1979).
45. M. Schluter, A. Zunger, G. P. Kerker, K. M. Ho, and M. L. Cohen, "Reliability of Pseudopotential Charge Densities," *Physical Review Letters* **42**, 540 (1979).
46. A. Zunger, "Contemporary Pseudopotentials: Simple Reliability Criteria," *J. Vac. Sci. Tech.* **16**, 1337-1348 (1979).

1980 (47-53)

47. A. Zunger, "Structural Stability of 495 Binary Compounds," *Physical Review Letters* **44**, 582-586 (1980).
48. A. Zunger, J. Perdew, and G. Oliver, "A Self-Interaction Corrected Approach to Many Electron Systems: Beyond the Local Spin Density Approximation," *Solid State Commun.* **34**, 933-936 (1980).
49. A. Zunger, "Ground State Properties of Crystalline Si in a Density Functional Pseudopotential Approach," *Phy. Rev. B* **21**, 4785-4790 (1980).
50. A. Zunger, "Nonlocal Pseudopotential Calculation of the Electronic Properties of Relaxed GaAs (110) Surface," *Phys. Rev. B* **22**, 959-969 (1980).
51. P. K. Lam, A. Zunger, and M. L. Cohen, "Analytic Representation for First Principles Pseudopotentials," *Phy. Rev. B* **22**, 1698-1708 (1980).

52. A. Zunger, "Spin Dependent Correlated Atomic Pseudopotentials," *Phys. Rev. B.* **22**, 649-662 (1980).
53. A. Zunger, "Systematization of the Crystal Structure of all Binary AB Compounds: A Pseudopotential Orbital Radii Approach," *Phys. Rev. B.* **22**, 5839-5872 (1980).

1981 (54-61)

54. A. Zunger, "A Pseudopotential Viewpoint of the Electronic and Structural Properties of Crystals," in *Structure and Bonding in Crystals*, edt. M. O'Keefe and A. Navrotsky, Academic Press, 1981, pp. 73-135.
55. J. P. Perdew and A. Zunger, "Self-Interaction Correction To Density Functional Approximations For Many Electron Systems," *Phys. Rev. B.* **23**, 5048-5079 (1981).
56. A. Zunger, "Pseudopotential and All-Electron Atomic Core Size Scales," *J. Chem. Phys.* **74**, 4209-4211 (1981).
57. J. P. Perdew, E. McMullen, and A. Zunger, "Density Functional Theory of Atomic Correlation Energies: A Simple Analytic Model and a Challenge," *Phys. Rev. A.* **23**, 2785-2789 (1981).
58. A. Zunger, "The Initial Stage of Formation of a Metal-Semiconductor Interface: Al on GaAs (110)," *J. Vac. Sci. Technol.* **19**, 690-692 (1981).
59. A. Zunger, "Phenomenology of the Crystal Structures of Transition Atom Binary Compounds," *Physical Review Letters* **47**, 1086 (1981).
60. U. Lindefelt and A. Zunger, "Quasi Bands in Green's Function Defect Models," *Phys. Rev. B.* **24**, 5913-5931 (1981).
61. A. Zunger, "Al on GaAs (110) Interface: The Possibility of Adatom Cluster Formation," *Phys. Rev. B.* **24**, 4372-4391 (1981).

1982 (62-67)

62. V. Singh and A. Zunger, "Phenomenology of Solid Solubilities and Ion Implantation Sites: An Orbital Radii Approach," *Phys. Rev. B.* **25**, 907-922 (1982).
63. V. Singh, U. Lindefelt, and A. Zunger, "Evaluation of Tight-Binding Models of Deep Defects in Semiconductors," *Phys. Rev. B.* **25**, 2781-2785 (1982).
64. P. Bendt and A. Zunger, "A New Approach for Solving the Density Functional Self-Consistent Field Problem," *Phys. Rev. B.* **26**, 3114-3137 (1982).

- 65. U. Lindefelt and A. Zunger, "The Quasi Band Crystal Field Method for Calculating the Electronic Structure of Localized Defects in Solids," *Phys. Rev. B* **26**, 846-895 (1982).
- 66. A. Zunger and U. Lindefelt, "Theory of Substitutional and Interstitial 3d Impurities in Silicon," *Phys. Rev. B. Rapid Communications* **26**, 5989-5992 (1982).
- 67. R. R. Daniels, A. D. Katnani, T. X. Zhao, G. Margaritondo, and A. Zunger, "The Initial Adsorption State for Al on GaAs (110) and Its Role in the Schottky Barrier Formation," *Physical Review Letters* **49**, 895-898 (1982).

1983 (68-80)

- 68. A. Zunger and U. Lindefelt, "Substitutional 3d Impurities in Silicon: A Self-Regulating System," *Solid State Commun.* **45**, 343-346 (1983).
- 69. A. Zunger and U. Lindefelt, "Electronic Structure of Substitutional 3d Transition Atom Impurities in Silicon," *Physica* **117B**, 185-187 (1983).
- 70. A. Zunger and U. Lindefelt, "Electronic Structure of Transition Atom Impurities in Semiconductors: Substitutional 3d Impurities in Silicon," *Phys. Rev. B* **27**, 1191-1227 (1983).
- 71. P. Bendt and A. Zunger, "Simultaneous Relaxation of Nuclear Geometries and Electronic Charge Densities in Electronic Structure Theories," *Physical Review Letters* **50**, 1684-1688 (1983).
- 72. V. Singh, A. Zunger, and U. Lindefelt, "A Reversal in the Order of Impurity Binding Energies with Atomic Energies," *Phys. Rev. B. Rapid Communications* **27**, 1420-1423 (1983).
- 73. V. A. Singh, U. Lindefelt, and A. Zunger, "Electronic Structure of Substitutional Chalcogen Impurities in Silicon," *Phys. Rev. B* **27**, 4909-4923 (1983).
- 74. A. Zunger, "The Origin of Schottky Barriers on the Cleavage Plane of III-V Semiconductors: Review of Some Recent Theoretical Work," *Thin Solid Films* **104**, 301-316 (1983).
- 75. A. Zunger, "One-Electron Broken Symmetry Approach to the Core Hole Spectra of Semiconductors," *Physical Review Letters* **50**, 1215-1218 (1983).
- 76. J. E. Jaffe and A. Zunger, "Anion Displacement and the Band Gap Anomaly in Ternary ABC₂ Chalcopyrite Semiconductors," *Phys. Rev. B. Rapid Communications* **27**, 5176-5179 (1983).
- 77. A. Zunger and J. E. Jaffe, "Structural Origin for Optical Bowing in Semiconductor Alloys," *Physical Review Letters* **51**, 662-665 (1983).

- 78.** J. Jaffe and A. Zunger, “Electronic Structure of CuAlS₂, CuGaS₂, CuAlSe₂, CuGaSe₂, and CuInSe₂,” *Phys. Rev. B* **28**, 5822-5847 (1983).
- 79.** T. X. Zhao, R. R. Daniels, A. D. Katnani, G. Margaritondo, and A. Zunger, “Schottky Barrier Formation and the Initial Metal-Atom Bonding State: InP(110)-Al vs GaAs(110)-Al,” *J. Vac. Sec. Technol. B* **1**, 610-612 (1983). See also R. R. Daniels, A. D. Katnani, T. X. Zhao, G. Margaritondo, and A. Zunger, *J. Vac. Sci. Technol. A* **1**, 617 (1983) for a short summary.
- 80.** A. Zunger, “Applicability of the Local Density Theory to Interstitial Transition Metal Impurities in Silicon,” *Phys. Rev. B. Rapid Communications* **28**, 3678-3631 (1983).

1984 (81-90)

- 81.** J. E. Jaffe and A. Zunger, “Theory of the Band Gap Anomaly in ABC₂ Chalcopyrite Semiconductors,” *Phys. Rev. B* **29**, 1882-1906 (1984).
- 82.** J. E. Jaffe and A. Zunger, “Electronic Structure of the Ternary Pnictide Semiconductors ZnSiP₂, ZnGeP₂, ZnSnP₂, ZnSiAs₂ and MgSiP₂,” *Phys. Rev. B* **30**, 741-756 (1984).
- 83.** A. Fazzio, M. Caldas, and A. Zunger, “Separation of Many and One Electron Effects in the Spectra of 3d Impurities in Semiconductors,” *Phys. Rev. B. Rapid Communications* **29**, 5999-6002 (1984).
- 84.** A. Fazzio, M. J. Caldas, and A. Zunger, “Many-Electron Multiplet Effects in the Spectra of 3d Impurities in Heteropolar Semiconductors,” *Phys. Rev. B* **30**, 3430-3455 (1984).
- 85.** A. Fazzio and A. Zunger, “Many Electron Multiplet Effects in the Optical Spectra of NiO, CoO and MnO,” *Solid State Commun.* **52**, 265-269 (1984).
- 86.** M. Caldas, A. Fazzio, and A. Zunger, “A Universal Trend in the Binding Energies of Deep Impurities,” *Appl. Phys. Letters* **45**, 671-673 (1984).
- 87.** H. Katayama-Yoshida and A. Zunger, “Localization and Magnetism of Interstitial Iron Impurity in Silicon,” *Physical Review Letters* **53**, 1256-1259 (1984).
- 88.** J. L. Martins and A. Zunger, “Bond Lengths Around Isovalent Impurities and in Semiconductor Alloys,” *Phys. Rev. B. Rapid Communications* **30**, 6217-6220 (1984).
- 89.** U. Linddefelt and A. Zunger, “Breathing Mode Relaxation Around Tetrahedral Interstitial 3d Impurities in Silicon,” *Phys. Rev. B. Rapid Communications* **30**, 1102-1105 (1984).
- 90.** U. Linddefelt and A. Zunger, “Interstitial Transition Atom Impurities in Silicon: Electronic Structure and Lattice Relaxation,” *J. Phys. C* **17**, 6047-6062 (1984).

1985 (91-108)

91. D. M. Wood and A. Zunger, "A New Method for Diagonalizing Large Matrices," *J. Phys. A* **18**, 1343-1359 (1985).
92. D. M. Wood, A. Zunger, and R. deGroot, "Electronic Structure of Filled Tetrahedral Compounds," *Phys. Rev. B. Rapid Communications* **31**, 2570-2573 (1985).
93. A. Zunger, "Composition Dependence of Deep Impurity Levels in Alloys," *Physical Review Letters* **54**, 848 (1985), (Comment).
94. A. Zunger, "Band Gap Anomaly in Tetrahedral Chalcopyrites and Optical Bowing in Binary Semiconductor Alloys," in *17th International Conference on the Physics of Semiconductors*, edits. J. Chadi and W. Harrison (Springer-Verlag, New York, 1985), pp. 997-1000.
95. U. Lindefelt and A. Zunger, "Symmetric Relaxation Around Interstitial 3d Impurities in Silicon," in *17th International Conference on the Physics of Semiconductors*, edits. J. Chadi and W. Harrison (Springer-Verlag, New York, 1985), pp. 729-732.
96. G. P. Srivastava, J. L. Martins, and A. Zunger, "Atomic Structure and Ordering in Semiconductor Alloys," *Phys. Rev. B Rapid Communications* **31**, 2561-2564 (1985). Erratum, *Phys. Rev. B* **38**, 12694 (1988).
97. V. A. Singh and A. Zunger, "Electronic Structure of Transition Atom Impurities in GaP," *Phys. Rev. B* **31**, 3729-3759 (1985).
98. M. Caldas, A. Fazzio, and A. Zunger, "Chemical Trends and Universalities in the Spectra of Transition Metal Impurities in Semiconductors," *J. Electron. Mat.* **14a**, 1035 (1985).
99. A. Zunger, "Theory of 3d Transition Atom Impurities in Semiconductors," *Annual Review of Material Science* **15**, 411-453 (1985).
100. H. Katayama-Yoshida and A. Zunger, "Hyperfine Interaction of the Iron Impurity Nuclei at the Tetrahedral Interstitial Site in Silicon," in *17th International Conference on the Physics of Semiconductors*, edits. J. Chadi and W. Harrison (Springer-Verlag, New York, 1985) pp. 733-736.
101. H. Katayama-Yoshida and A. Zunger, "Exchange-Correlation Induced Negative Effective U," *Physical Review Letters* **55**, 1618-1621 (1985).
102. H. Katayama-Yoshida and A. Zunger, "Chemical Trends in Ground and Excited State Properties of Interstitial 3D Impurities in Silicon," *Phys. Rev. B. Rapid Communications* **31**, 8317-8320 (1985).

- 103.** H. Katayama-Yoshida and A. Zunger, “Calculation of the Spin Polarized Electronic Structure of Interstitial Iron Impurity in Silicon,” *Phys. Rev. B*. **31**, 7877-7899 (1985).
- 104.** H. Katayama-Yoshida and A. Zunger, “Electronic and Magnetic Properties of Interstitial 3d Impurities in Silicon,” in *Microscopic Identification of Electronic Defects in Semiconductors*, edt. N. M. Johnson, S. G. Bishop, and G. D. Watkins, *Mat. Res. Soc. 46*, 111-116 (1985).
- 105.** J.L. Martins and A. Zunger, “Structural and Chemical Changes in Binary vs. Ternary Tetrahedral Semiconductors,” *Phys. Rev. B. Rapid Communications* **32**, 2689-2692 (1985).
- 106.** A.E. Carlson, D.M. Wood, and A. Zunger, “Electronic Structure of LiZnN and the Interstitial Insertion Rule,” *Phys. Rev. B. Rapid Communications* **32**, 1386-1389 (1985).
- 107.** A. Fazzio, M.J. Caldas, and A. Zunger, “Electronic Structure of Copper, Silver and Gold Impurities in Silicon,” *Phys. Rev. B*. **32**, 934-954 (1985).
- 108.** J. C. Phillips, A. Zunger, A. N. Bloch, and J. R. Chelikowsky, “Structural Stability of Crystalline Compounds,” *Physical Review Letters (Comment)* **55**, 260 (1985).

1986 (109-120)

- 109.** A. Zunger, “Ternary Semiconductors and Ordered Pseudobinary Alloys: Electronic Structure and Prediction of New Materials,” *Int. J. Quantum. Chem.* **19**, 629-653 (1986).
- 110.** D.M. Wood and A. Zunger, “Electronic Structure of Generic Semiconductors: Antifluorite Silicides and III-V's,” *Phys. Rev. B*. **34**, 4105-4120 (1986).
- 111.** A. Zunger, “Electronic Structure of 3d Transition Atom Impurities in Semiconductors,” in *Solid State Phys*, edit. F. Seitz, D. Turnbull, and H. Ehrenreich (Acad Press, NY) Vol. 39, 275-464 (1986).
- 112.** J.L. Martins and A. Zunger, “Ordering and Decomposition in Semiconductor Alloys,” *J. Mat. Res. Rapid Communications* **1**, 523-526 (1986).
- 113.** H. Katayama-Yoshida and Alex Zunger, “Prediction of a Low Spin Ground State in the GaAs:V²⁺ Impurity Systems,” *Phys. Rev. B. Rapid Communications* **33**, 2961-2964 (1986).
- 114.** S.-H. Wei and A. Zunger, “Electronic Structure and Phase Stability of LiZnAs: A Half Ionic and Half Covalent Tetrahedral Semiconductor,” *Physical Review Letters* **56**, 528-531 (1986).
- 115.** J. L. Martins and A. Zunger, “Stability of Ordered and Epitaxial Semiconductor Alloys,” *Physical Review Letters* **56**, 1400-1403 (1986).

- 116.** S. Froyen and A. Zunger, "Metastable Impurities in Semiconductors: Si:Mg and Si:Be," *Phys. Rev. B. Rapid Communications* **34** 7451-7454 (1986).
- 117.** S.-H. Wei and A. Zunger, "Alloy Stabilized Semiconducting and Magnetic Zincblende Phase of MnTe," *Physical Review Letters* **56**, 2391-2394 (1986).
- 118.** H. Katayama-Yoshida and A. Zunger, "Magnetic Properties of Interstitial 3d Impurities in Silicon," *J. Magnetism and Magnetic Materials* **54-57**, 1036-1038 (1986).
- 119.** J.E. Bernard and A. Zunger, "Optical Bowing in Zinc Chalcogenide Semiconductor Alloys," *Phys. Rev. B. Rapid Communications* **34**, 5992-5995 (1986).
- 120.** A.A. Mbaye, A. Zunger, and D.M. Wood, "Structural Stability and Selectivity of Thin Epitaxial Semiconductors," *Applied Physics Letters* **49**, 782-784 (1986).

1987 (121-139)

- 121.** A. A. Mbaye, L. G. Ferreira, and A. Zunger, "First Principles Calculations of Semiconductors Alloy Phase Diagrams," *Physical Review Letters* **58**, 49-52 (1987).
- 122.** A. Mbaye, and A. Zunger, "First Principles Calculation of Semiconductor Alloy Phase Diagrams: Ordered Ternary Compounds," in *Ternary and Multinary Compounds, Proc. 7th Int. Conf. MRS*, 1987, pp. 365-370.
- 123.** A. Zunger, "Order-Disorder Transformations in Ternary Tetrahedral Semiconductors," *Applied Physics Letters* **50**, 164-166 (1987).
- 124.** S.-H. Wei and A. Zunger, "Electronic Structure of M_3Sb -Type Filled Tetrahedral Semiconductors," *Phys. Rev. B.* **35**, 3952-3961 (1987).
- 125.** D. M. Wood, S.-H. Wei, and A. Zunger, "Thermodynamic Instability of Ultrathin Semiconductor Superlattices: The (001) $(GaAs)_1(AlAs)_1$ Structure," *Physical Review Letters* **58**, 1123-1126 (1987).
- 126.** J. Bernard and A. Zunger, "Electronic Structure of ZnS, ZnSe, ZnTe and their Pseudobinary Alloys," *Phys. Rev. B.* **36**, 3199-3228 (1987).
- 127.** S. Froyen, D. M. Wood, and A. Zunger, "New Optical Transitions in Strained Si_nGe_n Superlattices," *Phys. Rev. B. Rapid Communications* **36**, 4547-4550 (1987).
- 128.** D. M. Wood, S.-H. Wei, and A. Zunger, "Electronic Structure and Stability of $A^I B^{II} C^V$ Filled Tetrahedral Compounds," in *Ternary and Multinary Compounds, Proc. 7th Int. Conf. MRS*, 1987, pp. 523-532.

- 129.** S.H. Wei and A. Zunger, "Phase Stability and Band Structure of Semimagnetic $Cd_{1-x}Mn_xTe$ Semiconductor Alloy," in *Ternary and Multinary Comp, Proc. 7th Int. Con.*, MRS, 1987, pp. 485-490.
- 130.** S.-H. Wei and A. Zunger, "Total Energy and Band Structure Calculation for Semimagnetic $Cd_{1-x}Mn_xTe$ Semiconductor Alloy and Its Binary Constituents," *Phys. Rev. B* **35**, B 2340-2365 (1987).
- 131.** L. G. Ferreira, A. Mbaye, and A. Zunger, "Elastic and Chemical Interactions in Binary Alloy Phase Diagrams," *Phys. Rev. B. Rapid Communications* **35**, 6475-6478 (1987).
- 132.** S.-H. Wei, and A. Zunger, "Band Structure and Electronic Excitations in $Cd_{1-x}Mn_xTe$," *J. Mat. Res. Soc.* **89**, 197-202 (1987).
- 133.** S.-H. Wei and A. Zunger, "Role of d orbitals in Valence Band Offsets in Common-Anion Semiconductors," *Physical Review Letters* **59**, 144-147 (1987).
- 134** A. Zunger, "Theory of 3d Impurities in Semiconductors," in *18th International Conference in Semiconductors*, Ed. O. Engström, World Scientific, pp. 21-28 (1987).
- 135.** J. L. Martins and A. Zunger, "Theory of Ordering in Semiconductor Alloys," in *Ternary and Multinary Compounds, Proc. of the 7th Int. Conf.*, MRS, 1987, pp. 315-323.
- 136.** S.-H. Wei, A. A. Mbaye, L. G. Ferreira, and A. Zunger, "First-Principles Calculations of the Phase Diagrams of Noble Metals Cu-Au, Cu-Ag and Ag-Au," *Phys. Rev. B* **36**, 4163-4185 (1987).
- 137.** S. Froyen, D. M. Wood, and A. Zunger, "New Ordering-Induced Optical Transitions in Strained Si-Ge Superlattices," *Mat. Res. Soc.* **91**, 293-298 (1987).
- 138.** S.-H. Wei and A. Zunger, "Calculation of Valence Band Offset of Common-Anion Semiconductor Heterojunctions from Core Levels: The Role of Cation d Orbitals," *J. Vac. Sci. Technol B* **5**, 1239-1245 (1987).
- 139.** D. G. Kilday, G. Margaritondo, T. F. Ciszek, S. K. Deb, S.-H. Wei, and A. Zunger, "Common-Anion Rule and its Limits: Photoemission Studies of $CuIn_xGa_{1-x}Se_2/Ge$ and $Cu_xAg_{1-x}InSe_2/Ge$ Interfaces," *Phys. Rev. B. Rapid Communications* **36**, 9388-9391 (1987).

1988 (140-156)

- 140.** D. M. Wood, S.-H. Wei, and A. Zunger, "Stability and Electronic Structure of Ultrathin [001] $(GaAs)_m(AlAs)_m$ Superlattices," *Phys. Rev. B* **37**, 1342-1363 (1988).
- 141.** A. A. Mbaye, D. M. Wood, and A. Zunger, "Stability of Pseudomorphic Epitaxial Semiconductors and Their Alloys," *Phys. Rev. B* **37**, 3008-3024 (1988).

- 142.** L. G. Ferreira, A. A. Mbaye, and A. Zunger, “Chemical and Elastic Effects on Isostructural Phase Diagrams: the ε -G Approach,” *Phys. Rev. B.* **37**, 10547-10570 (1988).
- 143.** A. Zunger, S.-H. Wei, A. A. Mbaye, and L. G. Ferreira, “A Novel Viewpoint on the Cu-Au Phase Diagram: The Interplay Between Fixed Ising Energies and Elastic Effects,” *Acta. Metall.* **36**, 2239-2248 (1988).
- 144.** J. E. Bernard, S.-H. Wei, D. M. Wood, and A. Zunger, “Ordering-Induced Changes in the Optical Spectra of Semiconductor Alloys,” *Appl. Phys. Lett.* **52**, 311-313 (1988).
- 145.** S.-H. Wei and A. Zunger, “Electronic Structure of II-VI Compounds and Their Alloys: Role of Cation d Bands,” *J. Cryst. Growth* **86**, 1-7 (1988).
- 146.** J. E. Bernard and A. Zunger, “Ordered Vacancy Compound Semiconductors: Pseudocubic CdIn₂Se₄,” *Phys. Rev. B.* **37**, 6835-6856 (1988).
- 147.** S. Froyen, D. M. Wood, and A. Zunger, “Structural and Electronic Properties of Epitaxial Thin-Layer Si_nGe_n Superlattices,” *Phys. Rev. B.* **37**, 6893-6907 (1988).
- 148.** S.-H. Wei and A. Zunger, “Role of Metal d States in II-VI Semiconductors,” *Phys. Rev. B.* **37**, 8958-8981 (1988).
- 149.** S.H. Wei and A. Zunger, “Electronic Structure of Ultrathin (GaAs)_n(AlAs)_n [001] Superlattices and the Ga_{0.5}Al_{0.5}As Alloy,” *J. Appl. Phys.* **63**, 5794-5804 (1988).
- 150.** S.H. Wei and A. Zunger, “Electronic Structure and Stability of II-VI Semiconductors and Their Alloys: The Role of Metal d Bands,” *J. Vac. Sci. Technol.* **6A**, 2597-2611 (1988).
- 151.** D. M. Wood and A. Zunger, “Epitaxial Effects on Coherent Phase Diagrams,” *Physical Review Letters* **61**, 1501-1504 (1988).
- 152.** J. E. Bernard, L. G. Ferreira, S.-H. Wei, and A. Zunger, “Ordering of Isovalent Intersemiconductor Alloys,” *Phys. Rev. B. Rapid Communications* **38**, 6338-6341 (1988).
- 153.** S.-H. Wei and A. Zunger, “Thermodynamic Stability of (AlAs)_n(GaAs)_n Superlattices and the Random Al_{0.5}Ga_{0.5}As Alloy,” *Physical Review Letters* **61**, 1505-1508 (1988).
- 154.** S. Froyen, S.-H. Wei, and A. Zunger, “Epitaxy-Induced Structural Phase Transformations,” *Phys. Rev. B. Rapid Communications* **38**, 10124-10127 (1988).
- 155.** S.-H. Wei and A. Zunger, “(111)-Oriented (GaAs)_n(AlAs)_n Superlattices are Direct Band-Gap Materials for All n’s,” *Appl. Phys. Lett.* **53**, 2077-2079 (1988).

- 156.** D. M. Wood and A. Zunger, “Composition Pinning in Semiconductor Alloys,” *Phys. Rev. B. Rapid Communications* **38**, 12,756-12,759 (1988).

1989 (157-167)

- 157.** L. G. Ferreira, S.-H. Wei, and A. Zunger, “First-Principles Calculation of Alloy Phase Diagrams: The Renormalized Interaction Approach,” *Phys. Rev. B.* **40**, 3197-3231 (1989).
- 158.** S.-H. Wei and A. Zunger, “Band Gaps and Spin-Orbit Splitting of Ordered and Disordered $\text{Al}_x\text{Ga}_{1-x}\text{As}$ and $\text{GaAs}_x\text{Sb}_{1-x}$ Alloys,” *Phys. Rev. B.* **39**, 3279-3304 (1989).
- 159.** S.-H. Wei and A. Zunger, “Negative Spin-Orbit Bowing in Semiconductors Alloys,” *Phys. Rev. B. Rapid Communications* **39**, 6279-6289 (1989).
- 160.** N. E. Christensen, S.-H. Wei, and A. Zunger, “First-Principles Calculations of the Formation Energies of Ordered and Disordered Phases of AlAs-GaAs,” *Phys. Rev. B.* **40**, 1642-1646 (1989).
- 161.** A. Zunger and D. M. Wood, “Structural Phenomena in Coherent Epitaxial Solids,” *J. Cryst. Growth* **98**, 1-17 (1989).
- 162.** J. E. Bernard and A. Zunger, “Bonding Charge Density in GaAs,” *Physical Review Letters* (Comment) **62**, 2328 (1989).
- 163.** S. Froyen, D. M. Wood, and A. Zunger, “Electronic Structure and Optical Properties of Si-Ge Superlattices,” *Physical Review Letters* (Comment) **62**, 975 (1989).
- 164.** D. M. Wood and A. Zunger, “Epitaxial Effects on Coherent Phase Diagrams,” *Phys. Rev. B.* **40**, 4062-4089 (1989).
- 165.** A. Zunger, L. G. Ferreira, and S.-H. Wei, “First Principles theory of alloy Phase Diagrams,” *MRS Proceedings* **141**, 177 (1989).
- 166.** S. Froyen, D. M. Wood, and A. Zunger, “Electronic Structure of [110] Si-Ge Thin-layer Superlattices,” *Appl. Phys. Lett.* **54**, 2435-2437 (1989).
- 167.** S. Froyen, D. M. Wood, and A. Zunger, “Electronic Structure of Ultrathin Si_nGe_n Strained Superlattices: The Possibility of Direct Band Gaps,” *Thin Solid Films* **183**, 33-48 (1989).

1990 (168-180)

- 168.** Z. W. Lu, S.-H. Wei, and A. Zunger, “Absence of Volume Metastability in bcc Copper,” *Phys. Rev. B.* **41**, 2699-2703 (1990).

- 169.** S.-H. Wei, L. G. Ferreira, and A. Zunger, “First-Principles Calculation of Temperature-Composition Phase Diagrams of Semiconductor Alloys,” *Phys. Rev. B* **41**, 8240-8269 (1990).
- 170.** A. Zunger, S.-H. Wei, L. G. Ferreira, and J. E. Bernard, “Special Quasirandom Structures,” *Physical Review Letters* **65**, 353-356 (1990).
- 171.** S.-H. Wei and A. Zunger, “Instability of Diatomic Deuterium in fcc Palladium,” *J. Fusion Energy* **9**, 367-370 (1990).
- 172.** S.-H. Wei and A. Zunger, “Stability of Atomic and Diatomic Hydrogen in fcc Palladium,” *Solid State Commun.* **73**, 327-330 (1990).
- 173.** S.-H. Wei and A. Zunger, “Band Gap Narrowing in Ordered and Disordered Semiconductor Alloys,” *Appl. Phys. Lett.* **56**, 662-664 (1990).
- 174.** J. E. Bernard, R. G. Dandrea, L. G. Ferreira, S. Froyen, S.-H. Wei, and A. Zunger, “Ordering in Semiconductor Alloys,” *Appl. Phys. Lett.* **56**, 731-733 (1990).
- 175.** S.-H. Wei, L. G. Ferreira, J. E. Bernard, and A. Zunger, “Electronic Properties of Random Alloys: Special Quasirandom Structures,” *Phys. Rev. B* **42**, 9622-9649 (1990).
- 176.** R. G. Dandrea, J. E. Bernard, S.-H. Wei, and A. Zunger, “Stability of Coherently Strained Semiconductor Superlattices,” *Physical Review Letters* **64**, 36-39 (1990).
- 177.** R. G. Dandrea, S. Froyen, and A. Zunger, “Stability and Band Offsets of Heterovalent Superlattices: Si/GaP, Ge/GaAs and Si/GaAs,” *Phys. Rev. B. Rapid Communications* **42**, 3213-3216 (1990).
- 178.** R. G. Dandrea and A. Zunger, “Prediction of Direct Band Gaps in Monolayer (001) and (111) GaAs/GaP Superlattices,” *Appl. Phys. Lett.* **57**, 1031-1033 (1990).
- 179.** R. Magri, S.-H. Wei, and A. Zunger, “Ground State Structures and the Random State Energy of the Madelung Lattice,” *Phys. Rev. B. Rapid Communications* **42**, 11388-11391 (1990).
- 180.** K. C. Hass, L. C. Davis, and A. Zunger, “Electronic Structure of Random $\text{Al}_{0.5}\text{Ga}_{0.5}\text{As}$ Alloys: Test of the Special Quasirandom Structures Description,” *Phys. Rev. B. Rapid Communications* **42**, 3757-3760 (1990).

1991 (181-198)

- 181.** L. G. Ferreira, S.-H. Wei, and A. Zunger, “Stability, Electronic Structure and Phase Diagrams of Novel Inter-semiconductor Compounds,” *Int. J. Supercomput. Appl.* **5**, 34-56 (1991).

- 182** R. Magri and A. Zunger, “Thermodynamic Instability of Ordered (001) AlGaAs₂ in Bulk Form,” *Phys. Rev. B.* **43**, 1584 (1991).
- 183.** R. Magri, J. E. Bernard, and A. Zunger, “Predicting Structural Energies of Atomic Lattices,” *Phys. Rev. B.* **43**, 1593-1597 (1991).
- 184.** R. Magri, S. Froyen, and A. Zunger, “Electronic Structure and Density of States of Random AlGaAs, GaAsP, and InGaAs Semiconductor Alloys,” *Phys. Rev. B.* **44**, 7947-7964 (1991).
- 185.** R. Magri and A. Zunger, “A Real-space Description of the Semiconducting Band Gaps in Substitutional Systems,” *Phys. Rev. B.* **44**, 8672-8684 (1991).
- 186.** Z. W. Lu, S.-H. Wei, A. Zunger, and L. G. Ferreira, “Ground State Structures of Intermetallic Compounds: A First-Principles Ising Model,” *Solid State Commun.* **78**, 583-588 (1991).
- 187.** Z. W. Lu, S.-H. Wei, A. Zunger, S. Frota-Pessoa, and L. G. Ferreira, “First Principles Statistical Mechanics of Structural Stability of Intermetallic Compounds,” *Phys. Rev. B.* **44**, 512-544 (1991).
- 188.** Z. W. Lu, S.-H. Wei, and A. Zunger, “Electronic Structure of Random Ag_{0.5}Pd_{0.5} and Ag_{0.5}Au_{0.5} Alloys,” *Phys. Rev. B.* **44**, 10470-10484 (1991).
- 189.** Z. W. Lu, S.-H. Wei, and A. Zunger, “Ordering in Binary Late Transition Metal Alloys,” *Physical Review Letters* **66**, 1753-1756 (1991).
- 190.** Z. W. Lu, S.-H. Wei, and A. Zunger, “Large Lattice-Relaxation-Induced Electronic Level Shifts in Random Cu_{1-x}Pd_x Alloys,” *Phys. Rev. B. Rapid Communications* **44**, 3387-3390 (1991).
- 191.** S.-H. Wei and A. Zunger, “Disorder Effects on the Density of States of the II-VI Semiconductor Alloys HgCdTe, ZnCdTe, and HgZnTe,” *Phys. Rev. B.* **43**, 1662-1677 (1991).
- 192.** R. G. Dandrea and A. Zunger, “A First-Principles Study of Intervalley Mixing: Ultrathin GaAs/GaP Superlattices,” *Phys. Rev. B.* **43**, 8962-8989 (1991).
- 193.** R. Osorio, S. Froyen, and A. Zunger, “Structural Phase Transition in (GaAs)_{1-x}Ge_{2x} and (GaP)_{1-x}Si_{2x} Alloys: Test of the Bulk Thermodynamic Description,” *Phys. Rev. B.* **43**, 14055-14072 (1991).
- 194.** R. Osorio, S. Froyen, and A. Zunger, “Superlattice Energetics and Alloy Thermodynamics of GaAs/Ge,” *Solid State Commun.* **78**, 249-255 (1991).
- 195.** S. Froyen and A. Zunger, “Surface-Induced Ordering in GaInP,” *Physical Review Letters* **66**, 2132-2135 (1991).

- 196.** J. E. Bernard, S. Froyen, and A. Zunger, “Spontaneous Surface-Induced Long Range Order in $\text{Ga}_{0.5}\text{In}_{0.5}\text{P}$,” *Phys. Rev. B* **44**, 11178-11195 (1991). See also S. Froyen and A. Zunger, “Surface Reconstructions and Surface Energies of Monolayer Coverage Cation-Terminated $\text{Ga}_{0.5}\text{In}_{0.5}\text{P}$ (001) Surfaces,” *J. Vac. Sci. Technol. B* **9B**, 2176-2181 (1991).
- 197.** J. E. Bernard and A. Zunger, “Strain Energy and Stability in Si/Ge Compounds, Alloys, and Superlattices,” *Phys. Rev. B* **44**, 1663-1681 (1991).
- 198.** S.-H. Wei and A. Zunger, “Proposal for III-V Ordered Alloys with Infrared Band Gaps,” *Appl. Phys. Lett.* **58**, 2684-2686 (1991).

1992 (199-212)

- 199.** Z. W. Lu, S.-H. Wei, and A. Zunger, “Electronic Structure of Ordered and Disordered Cu_3Au and Cu_3Pd ,” *Phys. Rev. B* **45**, 10314-10330 (1992).
- 200.** Z. W. Lu, S.-H. Wei, and A. Zunger, “Theory of Bonding Charge Density in β NiAl,” *Acta Metallurgica* **40**, 2155-2165 (1992).
- 201.** Z. W. Lu and A. Zunger, “The Electronic Charge Distribution in Crystalline Silicon: Comparison of Ab-Initio Theory and Experiment,” *Acta. Cryst. A* **48**, 545-554 (1992).
- 202.** Z. W. Lu, S.-H. Wei, and A. Zunger, “Comment on the Origins of Compositional Order in NiPt Alloys,” *Physical Review Letters* (C) **68**, 1961 (1992).
- 203.** D. B. Laks and A. Zunger, “Theory of Interfacial Stability of Semiconductor Superlattices,” *Phys. Rev. B* **45**, 14177-14188 (1992).
- 204.** D. B. Laks, R. Magri, and A. Zunger, “Diamond-like Order in Zincblende Compounds,” *Solid State Commun.* **83**, 21-26 (1992).
- 205.** D.B. Laks, and A. Zunger, “Identity of Conduction Band Minimum in $(\text{AlAs})_1(\text{GaAs})_1$ Superlattices: Intermixing-induced Reversal of States,” *Phys. Rev. B. Rapid Communications* **45**, 11411-11414 (1992).
- 206.** D.B. Laks, L.G. Ferreira, S. Froyen, and A. Zunger, “An Efficient Cluster Expansion for Substitutional Systems,” *Phys. Rev. B* **46**, 12587-12605 (1992).
- 207.** D.B. Laks, S.-H. Wei, and A. Zunger, “Evolution of Alloy Properties with Long-Range Order,” *Physical Review Letters* **69**, 3766 (1992).
- 208.** S.-H. Wei, L. G. Ferreira, and A. Zunger, “First-Principles Calculation of Order-Disorder Transition in Chalcopyrite Semiconductors,” *Phys. Rev. B. Rapid Communications* **45** 2533-2536 (1992).

- 209.** R. Osorio, J. E. Bernard, S. Froyen, and A. Zunger, “Ordering Thermodynamics of Surface and Subsurface Layers in $\text{Ga}_{1-x}\text{In}_x\text{P}$ Alloy,” *Phys. Rev. B* **45**, 11173-11191 (1992). See also, “Thermodynamics of Surface-Induced Ordering in $\text{Ga}_{1-x}\text{In}_x\text{P}$ Alloys,” *J. Vac. Sci. Technol. B* **10**, 1683-1688 (1992), and *Physica Scripta T45*, 272 (1992).
- 210.** C.Y. Yeh, Z.W. Lu, S. Froyen, and A. Zunger, “Predictions and Systematizations of the Zincblende-Wurtzite Structural Energies in Binary Octet Compounds,” *Phys. Rev. B. Rapid Communications* **45**, 12130-12133 (1992).
- 211.** C.Y. Yeh, Z.W. Lu, S. Froyen, and A. Zunger, “The Zincblende-Wurtzite Polytypism in Semiconductors,” *Phys. Rev. B* **46**, 10086-10097 (1992).
- 212.** R.G. Dandrea, C.B. Duke, and A. Zunger, “Interfacial Atomic Structure and Band Offsets at Semiconductor Heterojunctions,” *J.Vac. Sci. Technol* **10B**, 1744-1753 (1992).

1993 (213-227)

- 213.** Z.W. Lu, A. Zunger, and M. Deutsch, “The Electronic Charge Distribution in Diamond, Silicon and Germanium,” *Phys. Rev. B* **47**, 9385-9410 (1993).
- 214.** Z.W. Lu, S.-H. Wei, and A. Zunger, “Relativity-Induced Ordering and Phase-Separation in Intermetallic Compounds,” *Europhysics Letters* **21**, 221-226 (1993).
- 215.** S.-H. Wei, D.B. Laks, and A. Zunger, “Dependence of the Optical Properties of Semiconductor Alloys on the Degree of Long-Range Order,” *Appl. Phys. Lett.* **62**, 1937-1939 (1993).
- 216.** A. Zunger, S. Wagner, and P.M. Petroff, “New Materials and Structures for Photovoltaics,” *J. Elect. Materials* **22**, 3-16 (1993).
- 217.** S.-H. Wei, and A. Zunger, “Electronic Origins of the Magnetic Phase Transitions in Zincblende Mn Chalcogenides,” *Phys. Rev. B* **48**, 6111-6115 (1993).
- 218.** S.-H. Wei, S.B. Zhang, and A. Zunger, “Off-Center Atomic Displacements in Zincblende Semiconductors,” *Physical Review Letters* **70**, 1639-1642 (1993); S.-H. Wei, S. B. Zhang, and A. Zunger, “Structural instability in zinc-blende semiconductors,” *Ferroelectrics* **155**, 127 (1994).
- 219.** R. Osorio, Z.W. Lu, S.-H. Wei, and A. Zunger, “First Principles Phase Diagrams of Pseudoternary Chalcopyrite/Zincblende Alloys,” *Phys. Rev. B. Rapid Communications* **47**, 9985-9988 (1993).
- 220.** L. Benguigui, R. Weil, E. Muranovich, A. Chack, E. Fredj, and A. Zunger, “Ferroelectric Properties of Cd Zn Te Solid Solutions,” *J. Appl. Phys.* **74**, 513-520 (1993); A. Eyal, R.

- Beserman, S.-H. Wei, A. Zunger, E. Maayan, O. Kreinin, J. Salzman, R. Westphalen, and K. Heime, "Influence of Ga concentration on the ordering process of $\text{Ga}_x\text{In}_{1-x}\text{P}$ grown on GaAs," *Jpn. J. Appl. Phys. Suppl.* **32-3**, 716 (1993).
- 221.** A. Nelson, C.R. Schwerdtfeger, S.H. Wei, and A. Zunger, "Theoretical and Experimental Studies of the ZnSe/CuInSe₂ Heterojunction Band Offsets," *Appl. Phys. Lett.* **62**, 2557-2559 (1993); A. J. Nelson, D. W. Niles, C. R. Schwerdtfeger, S.-H. Wei, A. Zunger, and H. Hochst, "Prediction and observation of II-VI/CuInSe₂ heterojunction band offsets," *Electron Spectrosc. and Relat. Phenom.* **68**, 185 (1994).
- 222.** S.H. Wei, and A. Zunger, "Band Offsets at the CdS/CuInSe₂ Heterojunction," *Appl. Phys. Lett.* **63**, 2549-2551 (1993).
- 223.** S.B. Zhang, and A. Zunger, "Prediction of Unusual Electronic Properties of Si Quantum Films," *Appl. Phys. Lett.* **63**, 1399-1401 (1993).
- 224.** S.B. Zhang, C.Y. Yeh and A. Zunger, "Electronic Structure of Semiconductor Quantum Films," *Phys. Rev. B.* **48**, 11,204 (1993).
- 225.** C.Y. Yeh, S.B. Zhang, and A. Zunger, "Identity of the Light Emitting States in Porous Silicon Wires," *Appl. Phys. Lett.* **63**, 3455 (1993)
- 226.** C.Y. Yeh, S.B. Zhang, S. Froyen, and A. Zunger, "Confinement Effects in Supported vs. Isolated Quantum Structures: A Study of Si(100) Film," *Supperlatt. & Microstruct.* **14**, 141-148 (1993).
- 227.** A. Zunger, "Prediction of New Semiconductor and Transition Metal Structures and their Properties," *Japan J. Appl. Phys. Suppl.* **32-3**, 14-21 (1993).
- 1994 (228-252)**
- 228.** A. Zunger, "First Principles Statistical Mechanics of Semiconductor Alloys and Intermetallic Compounds," in NATO Advanced Study Institute on *Statics and Dynamics of Alloy Phase Transformations*, edited by P. Turchi and A. Gonis, Plenum Press, New York, 361-419 (1994).
- 229.** C.Y. Yeh, S.B. Zhang, and A. Zunger, "Confinement, Surface and Chemisorption Effects on the Optical Properties of Si Quantum Wires," *Phys. Rev. B.* **50**, 14405-14415 (1994).
- 230.** C.Y. Yeh, S.B. Zhang, and A. Zunger, "Pressure Dependence of the Band Gap in Si Quantum Wires," *Appl. Phys. Lett.* **64**, 3545 (1994).
- 231.** C.Y. Yeh, S.-H. Wei, and A. Zunger, "Relationships Between the Band Gaps of the Zincblende and Wurtzite Modifications of Semiconductors," *Phys. Rev. B. Rapid Communications* **50**, 2715-2719 (1994).

- 232.** L.W. Wang, and A. Zunger, “Solving Schrodinger’s Equation Around a Desired Energy: Application to Si Quantum Dots,” *J. Chem. Phys.* (Letter section) **100**, 2394-2397 (1994).
- 233.** Wang, and A. Zunger, “Electronic Structure Pseudopotential Calculations of Large (~1000 atoms) Si Quantum Dots,” *J. Phys. Chem.* **98**, 2158-2165 (1994).
- 234.** L.W. Wang, and A. Zunger, “Large Scale Electronic Structure Calculations Using the Lanczos Method,” *Computational Mater. Sci.* **2**, 326-340 (1994).
- 235.** L.W. Wang and A. Zunger, “Dielectric Constants of Silicon Quantum Dots,” *Physical Review Letters* **73**, 1039-1041 (1994).
- 236.** Z.W. Lu, A. Zunger, and A.G. Fox, “Comparison of Experimental and Theoretical Electronic Charge Distributions in γ -TiAl,” *Acta Metall. Mater.* **42**, 3929-3943 (1994).
- 237.** Z. W. Lu, D.B. Laks, S.-H. Wei and A. Zunger, “First-Principles Simulated Annealing Study of Phase Transition and Short Range Order in Transition Metal and Semiconductor Alloys,” *Phys. Rev. B.* **50**, 6642-6661 (1994).
- 238.** Z.W. Lu, and A. Zunger, “Unequal Wavevectors in Short vs. Long Range Ordering in Intermetallic Compounds,” *Phys. Rev. B.* **50**, 6626-6636 (1994).
- 239.** S.-H. Wei, and A. Zunger, “Optical Properties of Zincblende Semiconductor Alloys: Effects of Epitaxial Strain and Atomic Ordering,” *Phys. Rev. B.* **49**, 14337-14351 (1994); S.-H. Wei and A. Zunger, “Optical Properties of $\text{Ga}_{0.5}\text{In}_{0.5}\text{P}$: Effects of strain and ordering,” in *Proceedings of the 22nd International Conference on the Physics of Semiconductors*, edited by D. J. Lockwood, (World Scientific, Singapore, 1995), p. 1268
- 240.** S.H. Wei, and A. Zunger, “Strain Effects on the Spectra of Spontaneously Ordered GaInP_2 ,” *Appl. Phys. Lett.* **64**, 757-759 (1994).
- 241.** S.H. Wei, and A. Zunger, “Optical Anisotropy and Spin Polarization in Ordered GaInP_2 ,” *Appl. Phys. Lett.* **64**, 1676-1678 (1994).
- 242.** A. Zunger, and S. Mahajan, “Atomic Ordering and Phase Separation in Epitaxial III-V Alloys,” in *Handbook of Semiconductors*, Vol 3, 2nd Edition, Elsevier, Amsterdam, P. 1399-1513 (1994).
- 243.** A. Zunger, “Structural Effects in Coherent Epitaxial Semiconductor Films,” in *Handbook of Crystal Growth*, Vol 3, edited by D.T.J. Hurle, Elsevier, Amsterdam, pp. 998-1047 (1994).
- 244.** J. E. Bernard, and A. Zunger, “Is there an Elastic Anomaly for a (001) Monolayer of InAs Embedded in GaAs?,” *Appl. Phys. Lett.* **65**, 165-167 (1994).

- 245.** C. Wolverton, A. Zunger and Z.W. Lu, “Long vs. Short Range Order in Ni₃V al Pd₃V,” *Phys. Rev. B. Rapid Communications* **49**, 16,058 - 16,061 (1994).
- 246.** C. Wolverton, and A. Zunger, “Comparison of Two Cluster Expansion Methods for the Energetics of Transition Metal Alloys,” *Phys. Rev. B.* **50**, 10548-10560 (1994).
- 247.** A. Franceschetti, S.-H. Wei, and A. Zunger, “Type II→Type I Transitions in GaX/InX (001) Superlattices (X=P, Sb) as a Function of Period,” *Phys. Rev. B. Rapid Communications* **50**, 8094-8097 (1994).
- 248.** A. Franceschetti, S.-H Wei and A. Zunger, “Absolute Deformation Potentials of Al, Si and NaCl,” *Phys. Rev. B.* **50**, 17,797-17801 (1994).
- 249.** A. Franceschetti, and A. Zunger, “Pressure dependence of optical transitions in ordered GaP/InP superlattices,” *Appl. Phys. Lett.* **65**, 2990-2993 (1994).
- 250.** A. Zunger, C. Y. Yeh, L. W. Wang and S. B. Zhang, “Electronic Structure of silicon quantum films, wires and dots: how good is the effective mass approximation?,” *Proc. Int. Conf. Phys. Semiconduct.* (Vancouver, Canada) edited by D. J. Lockwood, p. 1763, (1994).
- 251.** K. Mader and A. Zunger, “Effects of Atomic Clustering on the Optical Properties of III-V Alloys,” *Appl. Phys. Lett.* **64**, 2882-2884 (1994).
- 252.** K. Mader and A. Zunger, “Empirical atomic Pseudopotentials for AlAs/GaAs superlattices, alloys and Nanostructures,” *Phys. Rev. B.* **50** 17393-17405 (1994).

1995 (253-277)

- 253.** K. Mader and A. Zunger, “Short and Long Range Order Effects on the Electronic Properties of III-V Semiconductors,” *Phys. Rev. B.* **51**, 10462-10467 (1995).
- 254.** K. Mader, L. W. Wang, and A. Zunger, “Electronic Structure of Intentionally disordered AlAs/GaAs superlattices,” *Physical Review Letters* **74**, 2555-2559 (1995).
- 255.** K. Mader and A. Zunger, “Localization and Band Gap Pinning in Semiconductor Superlattices with Layer Thickness Fluctuations,” *Europhysics Letters* **31**, 107-112 (1995).
- 256.** K. Mader, L. W. Wang, and A. Zunger, “Electronic Consequences of Random Layer Thickness Fluctuations in AlAs/GaAs Superlattices,” *J. Appl. Phys.* **78**, 6639 (1995).
- 257.** L. W. Wang and A. Zunger, “LDA-derived Empirical Pseudopotentials,” *Phys. Rev. B.* **51**, 17398-17416 (1995).

- 258.** C. Wolverton and A. Zunger, “Short and long range order of the binary Madelung lattice,” *Phys. Rev. B.* **51**, 6876-6891 (1995).
- 259.** C. Wolverton and A. Zunger, “First Principles Theory of short range order and electronic excitations in Ni-V and Pd-V alloys,” *Phys. Rev. B.* **52**, 8813 (1995).
- 260.** C. Wolverton and A. Zunger, “An Ising-like description of structurally-relaxed ordered and disordered Alloys,” *Physical Review Letters* **75**, 3162 (1995).
- 261.** A. Franceschetti and A. Zunger, “Quantum Confinement-induced $\Gamma \rightarrow X$ transition in GaAs/GaAlAs quantum films, wires and dots,” *Phys. Rev. B.* **52**, 14,664 (1995).
- 262.** A. Franceschetti, S. H. Wei and A. Zunger, “Effects of Ordering on the Electron effective mass and strain deformation potential in GaInP₂: deficiencies of the k•p model,” *Phys. Rev. B.* **52**, 13,992 (1995).
- 263.** S. H.-Wei, A. Franceschetti, and A. Zunger, “E₁, E₂ and E'₀ transitions in ordered GaInP₂,” *Phys. Rev. B.* **51**, 13097 - 13102 (1995).
- 264.** S. H.-Wei, and A. Zunger, “Theory of Reflectance Difference Spectroscopy in Ordered III-V Semiconductor Alloys,” *Phys. Rev. B.* **51**, 14110-14114 (1995).
- 265.** A. Silverman, A. Zunger, R. Kalish and J. Adler, “Effects of configurational, positional and vibrational degrees of freedom on alloy phase-diagram: A Monte-Carlo study on GaInP₂,” *J. Phys. C. Cond. Mater.* **7**, 1167-1180 (1995). See Erratum in *J. Phys. C.* **7**, 5417 (1995).
- 266.** A. Silverman, A. Zunger, R. Kalish and J. Adler, “Correlated atomic displacements in the chemically random GaInP₂ alloy,” *Europhysics Letters* **31**, 373 (1995).
- 267.** A. Silverman, A. Zunger, R. Kalish and J. Adler, “The atomic-scale structure of disordered GaInP₂ alloys,” *Phys. Rev. B.* **51**, 10795-10816 (1995).
- 268.** Z. W. Lu, B. M. Klein and A. Zunger, “Ordering tendencies in Pd-Pt, Rh-Pt and Ag-Au alloys,” *J. Phase. Equilibria* **16**, 36 (1995).
- 269.** Z. W. Lu, B. M. Klein and A. Zunger, “Spin-polarization-induced structural selectivity in Pd₃X and Pt₃X (X=3d) compounds,” *Physical Review Letters* **75**, 1320-1323 (1995).
- 270.** Z. W. Lu, A. Zunger and M. Deutsch, “The Electronic charge Distribution in Crystalline Germanium,” *Phys. Rev. B.* **52**, 11,904-11,911 (1995).
- 271.** Z. W. Lu, A. Zunger and B. M. Klein, “Thermodynamic instability of Ag/Au, and Cu/Pd superlattices,” *J. Superlatt. & Microstruct.* **18**, 161-175 (1995).

- 272.** Z. W. Lu, B. M. Klein and A. Zunger, "Atomic short range order and alloy ordering tendencies in the Ag-Au system," *Modelling & Simulation in Mat. Sci.* **3**, 1-18 (1995).
- 273.** S.H. Wei and A. Zunger, "Band offsets and optical bowing of chalcopyrites and Zn-based II-VI alloys," *J. Appl. Phys.* **78**, 3846-3856, (1995).
- 274.** S. H. Wei and A. Zunger, "InAsSb/InAs: A Type I or a Type II band alignment," *Phys. Rev. B.* **52**, 12039-12044 (1995).
- 275.** S. B. Zhang, S. Froyen and A. Zunger, "Surface Dimerization induced CuPt_B vs. CuPt_A ordering in GaInP," *Appl. Physics Lett.* **67**, 3141-3143 (1995).
- 276.** S. B. Zhang and A. Zunger, "Structure and Formation Energy of Steps on GaAs (001) 2 x 4," *Mat. Sci. & Eng. B.* **30**, 127-136 (1995).
- 277.** S. B. Zhang, S. H. Wei and A. Zunger, "d-band excitations in II-VI semiconductors: a broken symmetry approach to the core hole," *Phys Rev. B.* **52**, 13975-13982 (1995).

1996 (278-300)

- 278.** L. W. Wang, K. Mader and A. Zunger, "Direct Calculation of the Transport Properties Of Disordered AlAs/GaAs Superlattices from the Electronic and Phonon Spectra," *Phys. Rev. B.* **53**, 2010-2019 (1996).
- 279.** S. B. Zhang and A. Zunger, "The Method of Linear Combination of Structural Motifs for Predicting Surface Step Energies: Application to GaAs (001)," *Phys. Rev. B.* **53**, 1343-1356 (1996).
- 280.** L.W. Wang and A. Zunger, "Pseudopotential Theory of Nanometer Silicon Quantum Dots," Chapter in *Studies in Surface Science and Catalysis*, Eds. P. V. Kamat and D. Meisel, Elsevier Science Vol. 103, p. 161-207 (1996).
- 281.** A. Zunger and L. W. Wang, "Theory of Silicon Nanostructures," *Appl. Surface Science*, **102**, 350-359 (1996).
- 282.** L. W. Wang and A. Zunger, "Pseudopotential calculations of nanoscale CdSe quantum dots," *Phys. Rev. B.* **53**, 9579-9582 (1996).
- 283.** A. Franceschetti and A. Zunger, "GaAs quantum-structures: Comparison between direct pseudopotential and single-band truncated-crystal calculations," *J. Chem. Phys.* **104**, 5572-5578 (1996).

- 284.** A. Franceschetti and A. Zunger, “Free-standing vs. AlAs-embedded GaAs quantum dots, wires and films: the emergence of zero confinement state,” *Appl. Phys. Lett.* **68**, 3455-3458 (1996).
- 285.** S. B. Zhang and A. Zunger, “Predicted Structures and stabilities of the Surface A Grooves and Double Bilayer Height Steps on the GaAs (001) 2 x 4 surface,” *J. Cryst. Growth* **163**, 113-121 (1996).
- 286.** D. M. Wood and A. Zunger, “Successes and failures of the k•p method: A direct assessment for GaAs/AlAs quantum structures,” *Phys. Rev. B.* **53**, 7949-7963 (1996).
- 287.** D. M. Wood, A. Zunger, and D. Gershoni, “Origins of k•p errors for (001) GaAs/AlAs heterostructures,” *Europhysics Letters* **33**, 383-389 (1996).
- 288.** S. H. Wei and A. Zunger, “Giant and Anomalously Composition dependent optical bowing coefficient in GaAsN alloys,” *Physical Review Letters* **76**, 664-667 (1996).
- 289.** S. Froyen and A. Zunger, “Surface segregation & surface ordering in III-V semiconductor Alloys,” *Phys. Rev. B.* **53**, 4570-4575 (1996).
- 290.** A. Zunger, “First Principles and Second Principles Pseudopotentials,” edited by J. R. Chelikowsky and S.G.Louie, Kluger Academic Publishers, Boston, 173-187 (1996).
- 291.** S.-H. Wei and A. Zunger, “Theoretical Studies of Chalcopyrite Alloys, Interfaces, and Ordered Compounds,” *Cryst. Res. Technol.* **31**, 81-88 (1996). A. Zunger and S.-H. Wei, “Electronic structure theory of chalcopyrite alloys, interfaces, and ordered vacancy compounds,” in *Proceedings of the 13th NREL PV Program Review*, edited by H. S. Ullal and C. E. Witt, (AIP, New York, 1995), p. 155.
- 292.** S.-H. Wei and A. Zunger, “Chemical trends in band offsets in Zn and Mn-based II-VIs: d-level pinning and offset compression,” *Phys. Rev. B. Rapid Communications* **53**, 10,457-10,460 (1996).
- 293.** (a) S.H. Wei, A. Franceschetti, and A. Zunger, “Dependence of optical properties of semiconductor alloys on long range order, strain, and pressure,” in *Optoelectronic Materials - Ordering, Composition Modulation, and Self-Assembled Structures*, edited by E. D. Jones, A. Mascarenhas, P. Petroff, and R. Bhat, (Matrl. Res. Society, Pittsburgh, 1996), **417**, 3-17; (b) A. Franceschetti, S.-H. Wei and A. Zunger, “Prediction of new fingerprints of ordering in GaInP₂,” *ibid* **417**, 103-108 (1996); (c) S.B. Zhang, S. Froyen and A. Zunger, “Theory of Surface Dimerization-induced ordering in GaInP alloys,” *ibid* **417**, 43-48 (1996).
- 294.** L. W. Wang and A. Zunger, “Pseudopotential-based multiband k•p method for 250,000-atom nanostructure systems,” *Phys. Rev. B.* **54**, 11417-11435 (1996).

- 295. S. B. Zhang and A. Zunger, "Structure of the As vacancy on GaAs (110) surfaces," *Physical Review Letters* **77**, 119-122 (1996).
- 296. C. Wolverton, S. Froyen, S.H. Wei and A. Zunger, "Point-charge electrostatics in Disordered Alloys," *Phys. Rev. B* **54**, 7843-7856 (1996).
- 297. S. Froyen, A. Zunger and A. Mascarenhas, "Polarization fields and band offsets in GaInP/GaAs and ordered/disordered superlattices," *Appl. Phys. Lett.* **68**, 2852-2854 (1996).
- 298. A. Zunger, "Pseudopotential Theory of Semiconductor Quantum Dots, Wires, and Films," in *23rd Conference on the Physics of Semiconductors*, Edited by M. Scheffler and R. Zimmermann, World Science, Singapore, Vol. 2, p.1341-1348 (1996).
- 299. S.H. Wei and A. Zunger, "Valence Band Splittings and Band Offsets in AlN, GaN, and InN," *Appl. Phys. Lett.* **69**, 2719-2721 (1996).
- 300. L. Bellaiche, S.H. Wei and A. Zunger, "Localization and Percolation in Semiconductor Alloys: GaAsN vs. GaAsP," *Phys. Rev. B* **54**, 17568-17576 (1996).

1997 (301-319)

- 301. L. Bellaiche, S.H. Wei and Alex Zunger, "Composition-dependence of Interband Transition Intensities in Isovalent Semiconductor Alloys: GaPN vs. GaPAs," *Phys. Rev. B* **56**, 10233-10240 (1997).
- 302. L. Bellaiche, S. H. Wei and A. Zunger, "Band gaps of GaPN and GaAsN Alloys," *Appl. Phys. Lett.* **70**, 3558-3560 (1997).
- 303. L. Bellaiche, S.H. Wei and A. Zunger, "Bond Length Distribution in Tetrahedral vs. Octahedral Semiconductor Alloys: the Case of GaInN," *Phys. Rev. B* **56**, 13872-13877 (1997).
- 304. S.B. Zhang and A. Zunger, "Surface-reconstruction-enhanced Solubility of N, P, As, and Sb in III-V Semiconductors," *Appl. Phys. Lett.* **71**, 677-679 (1997).
- 305. S.H. Wei and A. Zunger, "Electronic and Structural Anomalies in Lead Chalcogenides," *Phys. Rev. B* **55**, 13605-13610 (1997).
- 306. S.B. Zhang, S.H. Wei and A. Zunger, "Stabilization of Ternary Compounds via Ordered Arrays of Defect Pairs," *Physical Review Letters* **78**, 4059-4062 (1997).
- 307. S.H. Wei, S.B. Zhang and A. Zunger, "Why is Heavily-defected CuInSe₂ a Good Opto-electronic Material: Defect Physics in CuInSe₂," *Int. Conf. Ternary & Multinary Compounds* (1997).

- 308.** A. Zunger, “Spontaneous Atomic Ordering in Semiconductor Alloys: Causes, Carriers, and Consequences,” *MRS Bulletin Special Issue* **22**, 20-26 (1997).
- 309.** L.W. Wang and A. Zunger, “The Magnitude and Size Scaling of Intervalley Coupling in Semiconductor Alloys and Superlattices,” *Phys. Rev. B.* **56**, 12395-12403 (1997).
- 310.** H. Fu and A. Zunger, “Local-density-derived Semiempirical Nonlocal Pseudopotentials for InP with Applications to Large Quantum Dots,” *Phys. Rev. B.* **55**, 1642-1653 (1997).
- 311.** H. Fu and A. Zunger, “InP Quantum Dots: Electronic Structure, Surface Effects, and the Redshifted Emission,” *Phys. Rev. B.* **56**, 1496-1508 (1997).
- 312.** O.I. Miñoz, H.M. Cheong, H. Fu, A. Zunger, J.R. Sprague, A. Mascarenhas, and A.J. Nozik, “Size-dependent Spectroscopy of InP Quantum Dots,” *J. Phys. Chem. B* **101**, 4904-4912 (1997).
- 313.** H. Fu, L.W. Wang and A. Zunger, “Comparison of the k•p and the direct diagonalization approaches for describing the electronic structure of quantum dots,” *Appl. Phys. Lett.* **71**, 3433-3435 (1997); H. Fu, L. W. Wang and A. Zunger, “Response to ‘Comment on comparison of the k•p and the direct diagonalization approaches for describing the electronic structure of quantum dots,’” *Appl. Phys. Lett* **73**, 115 (1998).
- 314.** A. Franceschetti and A. Zunger, “Direct Pseudopotential Calculation of Exciton Coulomb and Exchange Energies in Semiconductor Quantum Dots,” *Physical Review Letters* **78**, 915-918 (1997).
- 315.** L.W. Wang, A. Franceschetti and A. Zunger, “Million-Atom Pseudopotential Calculation of Γ -X Mixing in GaAs/AlAs Superlattices and Quantum Dots,” *Physical Review Letters* **78**, 2819-2822 (1997).
- 316.** C. Wolverton and A. Zunger, “Ni-Au: A testing ground for theories of phase stability,” *Comput. Mater. Sci.* **8**, 107-121 (1997).
- 317.** C. Wolverton and A. Zunger, “Invertible and non-invertible Alloys Ising Problems,” *Solid State Commun.* **101**, 519 (1997).
- 318.** S.-H. Wei and A. Zunger, “Point-Ion vs. Density Functional Calculations of Electric-Field Gradients in Ordered GaInP₂,” *J. Phys. Chem.* **107**, 1931 (1997).
- 319.** J. Kim, L.W. Wang and A. Zunger, “Prediction of charge separation in GaAs/AlAs Cylindrical nanostructures,” *Phys. Rev. B. Rapid Communications* **56**, R15541 (1997).

1998 (320 - 352)

- 320.** L.G. Ferreira, C. Wolverton and A. Zunger, “Evaluating and improving the cluster variation method entropy functional for Ising alloys,” *J. Chem. Phys.* **108**, 2912 (1998).
- 321.** V. Ozolins, C. Wolverton and A. Zunger, “Comment on ‘Anomalous Temperature Dependence of the X-ray Diffuse Scattering Intensity of Cu₃Au,’” *Physical Review Letters* **79**, 955 (1998) (Comment).
- 322.** C. Wolverton, V. Ozolins, and A. Zunger, “First-Principles Theory of Short-range Order in Size-mismatched Metal Alloys: Cu-Au, Cu-Ag, and Ni-Au,” *Phys. Rev. B.* **57**, 4332 (1998).
- 323.** V. Ozolins, C. Wolverton and A. Zunger, “Cu-Au, Ag-Au, Cu-Ag and Ni-Au intermetallics: First-principles study of phase diagrams and structures,” *Phys. Rev. B.* **57**, 6427 (1998).
- 324.** V. Ozolins, C. Wolverton and A. Zunger, “Effects of an harmonic strain on phase stability of epitaxial films and superlattices: applications to noble metals,” *Phys. Rev. B.* **57**, 4816 (1998).
- 325.** V. Ozolins, C. Wolverton and A. Zunger, “Strain-induced shift in the elastically soft direction of epitaxially grown fcc metals,” *Appl. Phys. Lett.* **72**, 427 (1998).
- 326.** V. Ozolins and A. Zunger, “First-Principles Theory of the Evolution of Vibrational Properties with Long-range Order in GaInP₂,” *Phys. Rev. B. Rapid Communications* **57**, R9404 (1998).
- 327.** S.-H. Wei and A. Zunger, “Fingerprints of CuPt ordering in III-V Semiconductor Alloys: Valence Band Splitting, Band Gap Reduction, and X-Ray Structure Factors,” *Phys. Rev. B.* **57**, 8983 (1998).
- 328.** S.B. Zhang, S.H. Wei and A. Zunger, “A Phenomenological Model for Systematization and Prediction of Doping Limits in II-VI and I-III-VI₂ Compounds,” *J. Appl. Phys.* **83**, 3192 (1998).
- 329.** S.B. Zhang, S.H. Wei, A. Zunger and H. Katayama-Yoshida, “Defect Physics of the CuInSe₂ Chalcopyrite Semiconductor,” *Phys. Rev. B.* **57**, 9642 (1998). S.H. Wei, S.B. Zhang and A. Zunger, “Why is Heavily-Defected CuInSe₂ a Good Opto-Electronic Material: Defect Physics in CuInSe₂ (1998),” R.D. Tomlinson, A.E., Hill, R.D. Pilkington, *Proc. of the 11th Int'l Conf. on Ternary and Multinary Compounds*, ICTMC-11, 8-12, *Salford Institute of Physics Conf. Series* #152, pp. 765-771.
- 330.** C. Pryor, J. Kim, L.W. Wang, A. Williamson and A. Zunger, “Comparison of two methods for describing the strain profiles in quantum dots,” *J. Appl. Phys.* **83**, 2548 (1998).

331. A.J. Williamson, A. Zunger, and A. Canning, "Prediction of a strain-induced conduction-band minimum in embedded quantum dots," *Phys. Rev. B. Rapid Communications* **57**, R4253 (1998).
332. J. Kim, L.W. Wang and A. Zunger, "Comparison of the electronic structure of InAs/GaAs pyramidal quantum dots with different facet orientations," *Phys. Rev. B. Rapid Communications* **57**, R9408 (1998).
333. L.W. Wang, L. Bellaiche, S.H. Wei and A. Zunger, "The 'Majority Representation' of Alloy Electronic States," *Physical Review Letters* **80**, 4725 (1998).
334. H. Fu, L.W. Wang, and A. Zunger, "On the applicability of the k•p method to the electronic structure of quantum dots," *Phys. Rev. B.* **57**, 9971 (1998).
335. H. Fu and A. Zunger, "Quantum-size effects on the pressure-induced direct-to-indirect band gap transition in InP quantum dots," *Physical Review Letters* **80**, 5397 (1998).
336. H. Fu and A. Zunger, "Excitons in InP Quantum Dots," *Phys. Rev. B. Rapid Communication* **57**, R15064 (1998).
337. A. Franceschetti, L.W. Wang, H. Fu and A. Zunger, "Short-range vs. long-range electron-hole exchange interactions in semiconductor quantum dots," *Phys. Rev. B. Rapid Communication* **58**, R13,370 (1998).
338. A. Zunger, "Electronic Structure Theory of Semiconductor Quantum Dots," *MRS Bulletin Special Issue* **23**, 35 (1998).
339. L.W. Wang and A. Zunger, "High Energy Excitonic Transitions in CdSe Quantum Dots," *J. Phys. Chem. (Letter section)* **102** 6449 (1998).
340. A. J. Williamson and A. Zunger, "Effect of interfacial states on the binding energies of electrons and holes in InAs/GaAs quantum dots," *Phys. Rev. B.* **58**, 6724-6727 (1998).
341. C. Wolverton and A. Zunger, "Prediction of Li Intercalation and Battery Voltages in Cubic vs. Rhombohedral Li_xCoO_2 ," *J. Electrochem. Soc.* **145**, 2424 (1998).
342. C. Wolverton and A. Zunger, "Cation- and vacancy-ordering in Li_xCoO_2 ," *Phys. Rev. B.* **57**, 2242 (1998).
343. C. Wolverton and A. Zunger, "First-principles theory of vacancy order-disorder and intercalation battery voltages in Li_xCoO_2 ," *Physical Review Letters* **81**, 606 (1998). C. Wolverton and A. Zunger, "First-Principles Theory of Cation and Intercalation Ordering in Li_xCoO_2 (1998)," D.S. Ginley, et al., eds., *Materials Research Society Symposium Proc. Vol. 496*, Warrendale, PA, pp. 77-88.

- 344. V. Ozolins, C. Wolverton and A. Zunger, "First-principles theory of vibrational effects on the phase stability of Cu-Au compounds and alloys," *Phys. Rev. B. Rapid Communications* **58**, R5879 (1998).
- 345. A. Zunger, "Predictions of Electronic Materials and Their Properties," in *Current Opinion in Solid State & Materials Science* **3**, 32 (1998).
- 346. S.H. Wei, and A. Zunger, "Calculated natural band offsets of all II-VI and III-V semiconductors," *Appl. Phys. Lett.* **72**, 2011 (1998).
- 347. S.H. Wei, S.B. Zhang and A. Zunger, "The effects of Ga addition to CuInSe₂ on its electronic, structural and defect properties," *Appl. Phys. Lett.* **72**, 3199 (1998).
- 348. S.H. Wei, A. Zunger, I.H. Choi and P.Y. Yu, "Trends in band gap pressure coefficients in chalcopyrite semiconductors," *Phys. Rev. B. Rapid Communications* **58**, R1710 (1998).
- 349. T. Mattila, L. Bellaiche, L.W. Wang and A. Zunger, "Electronic Structure induced by lateral composition modulation in InGaAs alloys," *Appl. Phys. Lett.* **72**, 2144 (1998).
- 350. L. Bellaiche and A. Zunger, "Effect of atomic short range order on the electronic and optical properties of GaAsN, GaInN and GaInAs alloys," *Phys. Rev. B.* **57**, 4425 (1998).
- 351. T. Mattila and A. Zunger, "Deep electronic gap levels induced by isovalent P and As impurities in GaN," *Phys. Rev. B.* **58**, 1367 (1998).
- 352. H. X. Fu, V. Ozolins and A. Zunger, "Phonons in GaP quantum dots," *Phys. Rev. B.* **59**, 7881-2887 (1998).

1999 (353-379)

- 353. L. W. Wang, J. Kim and A. Zunger, "Electronic structures of [110] faceted 'self-assembled' Pyrmidal InAs/GaAs quantum dots," *Phys. Rev. B.* **59**, 5678-5687 (1999).
- 354. H. Fu, L. W. Wang and A. Zunger, "Excitonic exchange splitting in bulk semiconductors," *Phys. Rev. B.* **59**, 5568-5574 (1999).
- 355. T. Mattila and A. Zunger, "P-P and As-As isovalent impurity pairs in GaN," *Phys. Rev. B.* **59**, 9943-9953 (1999).
- 356. T. Mattila and A. Zunger, "Predicted bond length variation in Wurtzite and Zinc-blende InGaN and AlGaN Alloys," *J. Appl. Phys.* **85**, 160-167 (1999).

- 357.** T. Mattila, S.H. Wei and A. Zunger, “Electronic structure of lateral composition modulation in semiconductor alloys,” *Phys. Rev. B*. **59**, 15,270 (1999).
- 358.** L.W. Wang, S.H. Wei, T. Mattila, A. Zunger, I. Vurgaftman and J. R. Meyer, “Multi-band coupling and electronic structure of InAs/GaSb superlattices,” *Phys. Rev. B*. **60**, 5590-5596, (1999).
- 359.** L. Bellaiche, T. Mattila, L.W. Wang, S.H. Wei and A. Zunger, “Resonant hole localization and anomalous optical bowing in InGaN alloys,” *Appl. Phys. Lett.* **74**, 1842-1844 (1999).
- 360.** T. Mattila, S.H. Wei and A. Zunger, “Electronic structure of sequence mutations in ordered GaInP₂,” *Physical Review Letters* **83**, 2010-2013 (1999).
- 361.** T. Mattila, S.H. Wei and A. Zunger, “Localization and anticrossing of electron levels in GaAsN alloys,” *Phys. Rev. B. Rapid Communication* **60**, R11245-R11248 (1999).
- 362.** A. J. Williamson and A. Zunger, “InAs quantum dots: predicted electronic structure of free-standing versus GaAs-embedded structures,” *Phys. Rev. B*. **59**, 15819-15824 (1999).
- 363.** A.J. Williamson, A. Franceschetti, H. Fu, L.W. Wang and A. Zunger, “Indirect band gaps in quantum dots made of direct-gap bulk materials,” *J. Elect. Mater.* **28**, 414-425 (1999).
- 364.** A. Zunger, “How to describe the electronic structure of semiconductor quantum dots,” *Electrochem. Soc. Proc.* **98-19**, 259-268 (1999).
- 365.** L.W. Wang and A. Zunger, “A linear-combination-of-bulk-bands method for large-scale electronic structure calculations on strained heterostructures,” *Phys. Rev. B*. **59**, 15806-15818 (1999).
- 366.** F. Reboreda, A. Franceschetti and A. Zunger, “Excitonic transitions and exchange-splitting in Si quantum-dots,” *App. Phys. Lett.* **75**, 2972 (1999).
- 367.** S.H. Wei, S.B. Zhang and A. Zunger, “Band structure and stability of zincblende-based semiconductor polytypes,” *Phys. Rev. B. Rapid Communication* **59**, R2478-2481 (1999).
- 368.** S.H. Wei and A. Zunger, “Predicted band gap pressure coefficients of all diamond and zincblende semiconductors,” *Phys. Rev. B*. **60**, 5404-5411 (1999).
- 369.** S.H. Wei, S.B. Zhang and A. Zunger, “Effects of Na on the electrical and structural properties of CuInSe₂,” *J. Appl. Phys.* **85**, 7214-7218 (1999).
- 370.** C. Wolverton and A. Zunger, “Magnetic destabilization of Ni₇Al,” *Phys. Rev. B*. **59**, 12,165-12,168 (1999).

- 371. L.G. Ferreira, V. Ozolins and A. Zunger, “Fitting accurate interatomic pair potentials for bulk metallic alloys using unrelaxed LDA energies,” *Phys. Rev. B* **60**, 1687-1696 (1999).
- 372. V. Ozolins and A. Zunger, “Theory of systematic absence of NaCl-Type (beta-Sn Type) high pressure phases in covalent (ionic) semiconductors,” *Physical Review Letters* **82**, 767 (1999).
- 373. K. Kim, V. Ozolins and A. Zunger, “Instability of the high-pressure CsCl structure in most III-V semiconductors,” *Phys. Rev. B. Rapid Communication* **60**, R8449 (1999).
- 374. A. Franceschetti and A. Zunger, “The inverse band structure problem: find the atomic configuration with given electronic properties,” *Nature* **402**, 60 (1999).
- 375. A. Franceschetti, H. Fu, L.W. Wang and A. Zunger, “Many-body pseudopotential theory of excitons in InP and CdSe quantum dots,” *Phys. Rev. B* **60**, 1819 (1999).
- 376. A. Franceschetti, L.W. Wang and A. Zunger, “Comment on quantum confinement and optical band gaps of Si nanocrystals,” *Physical Review Letters* **83**, 1269 (1999).
- 377. S. Müller, C. Wolverton, L.W. Wang and A. Zunger, “Coherent Phase-Stability in Al-Zn and Al-Cu Fcc Alloys: The Role of the Instability of fcc Zn,” *Phys. Rev. B* **60**, 16,448-16,462 (1999).
- 378. S.B. Zhang, S-H Wei and A. Zunger, “Overcoming Doping Bottlenecks in Semiconductors and Wide-Gap Materials,” *Physica-B* **273-274**, 976-980 (1999).
- 379. A. Zunger, “Anomalous Behavior of the Nitride Alloys,” *Phys. Stat. Sol. B* **216**, 117-123 (1999).

2000 (380-397)

- 380. A.J. Williamson and A. Zunger, “A pseudopotential study of electron-hole excitations in colloidal, free-standing InAs quantum dots,” *Phys. Rev. B* **61**, 1978-1991 (2000).
- 381. F.A. Reboreda, A. Franceschetti and A. Zunger, “Dark excitons due to direct Coulomb interactions in Si quantum dots,” *Phys. Rev. B* **61**, 13,073 (2000).
- 382. S.B. Zhang, S.H. Wei and A. Zunger, “The microscopic origin of the phenomenological doping-limit-rule in semiconductors and insulators,” *Physical Review Letters* **84**, 1232-1235 (2000).
- 383. J.H. Cho, S.B. Zhang and A. Zunger, “Indium-indium pair correlation and surface segregation in InGaAs alloys,” *Physical Review Letters* **84**, 3654 (2000).

- 384.** L.W. Wang, A.J. Williamson, A. Zunger, H. Jiang and J. Singh, “Comparison of the k•p and Direct Diagnolization Approaches to the Electronic Structure of InAs/GaAs Quantum Dots,” *App. Phys. Lett.* **76**, 339-341 (2000).
- 385.** S-H Wei, S.B. Zhang and A. Zunger, “First-principles Calculation of Band Offsets, Optical Bowings, and Defects in CdS, CdSe, CdTe and their Alloys,” *J. Appl. Phys.* **87**, 1304-1311 (2000).
- 386.** C. Wolverton, V. Ozolins and A. Zunger, “Short-range Order Types in Metallic Alloys: A Reflection of Coherent Phase Stability,” *J. Phys. C* **12**, 2749 (2000).
- 387.** A. Franceschetti, A. Williamson and A. Zunger, “Addition Spectra of Quantum Dots: The Role of Dielectric Mismatch,” *J. Phys. Chem (Letter Section)* **104**, 3398 (2000).
- 388.** A. Franceschetti and A. Zunger, “Pseudopotential Calculations of Electron and Hole Addition Spectra of InAs, InP and Si Quantum Dots,” *Phys. Rev. B.* **62**, 2614 (2000).
- 389.** A. Franceschetti and A. Zunger, “Addition Energies and Quasi-Particle gaps of CdSe nanocrystals,” *Appl. Phys. Lett.*, **76**, 1731 (2000).
- 390.** A. Franceschetti and A. Zunger, “Hund’s Rule, Spin-Blocade and the Aufbau Principle in Strongly-Confining Semiconductor Quantum Dots,” *Europhysics Letters* **50**, 243 (2000).
- 391.** A. Franceschetti and A. Zunger, “Optical transitions in charged CdSe quantum dots,” *Physical Review B. Rapid Communications* **62**, R16287 (2000).
- 392.** R. Magri, L.W. Wang , A. Zunger, I. Vurgaftman and J.R. Meyer, “Anticrossing Semiconducting Band Gap in Nominally Semimetallic InAs/GaSb Superlattices,” *Phys. Rev. B.* **61**, 10,235 (2000).
- 393.** R. Magri and A. Zunger, “Anticrossing and coupling of light-hole and heavy-hole states in (001) GaAs/GaAlAs heterostructures,” *Phys. Rev. B.* **62**, 10,364 (2000).
- 394.** A.J. Williamson, L.W. Wang and A. Zunger, “Theoretical Interpretation of the Experimental Electronic Structure of Lens-Shaped, Self-Assembled InAs/GaAs Quantum-Dots,” *Phys. Review B.* **62**, 12,963 (2000).
- 395.** A. Canning, L.W. Wang, A. Williamson and A. Zunger, “Parallel Empirical Pseudopotential Electronic Structure Calculations for Million Atom Systems, ” *J. Comput. Phys.* **160**, 29 (2000).
- 396.** G. Hart and A. Zunger, “Electronic Structure of BAs and Boride III-V Alloys,” *Physical Review B* **62**, 13522 (2000).

- 397.** F.A. Reboredo and A. Zunger, “L-to-X crossover in the conduction band minimum of Ge quantum dots,” *Physical Review B. Rapid Communication* **62**, R2275 (2000).

2001 (398 - 424)

- 398.** A. Franceschetti and A. Zunger, “Exciton dissociation and interdot transport in CdSe quantum-dot molecules,” *Physical Review B* **63**, Article Number 153,304 (2001).
- 399.** A.J. Williamson, A. Franceschetti and A. Zunger, “Multi-Excitons in Self-Assembled InAs/GaAs Dots: A Pseudopotential Many-Body Approach,” *Europhysics Letters* **53**, 59 (2001).
- 400.** F. Reboredo, S.B. Zhang and A. Zunger, “Hydrogen-Induced Instability on the Flat (100) Si Surface via Steric Repulsion,” *Physical Review B* **63**, Article No.125,316 (2001).
- 401.** F.A. Reboredo and A. Zunger, “Surface-passivation-induced optical changes in Ge quantum-dots,” *Physical Review B* **63**, Article No.235,314 (2001).
- 402.** J. Shumway, A. Franceschetti and A. Zunger, “Correlation vs. mean-field contributions to excitons, multi-excitons, and charging energies in semiconductor quantum dots,” *Physical Review B* **63**, Article No.155,316 (2001).
- 403.** J. Shumway, A.J. Williamson, A. Zunger, A. Passaes, M. DeGiorgi, R. Cingolani, M. Catalano and P. Crozier, "Electronic structure consequences of In/Ga composition variations in self-assembled InGaAs/GaAs alloy quantum dots," *Physical Review B* **64**, Article No. 125,302 (2001).
- 404.** Alex Zunger, “Pseudopotential Theory of Semiconductor Quantum-Dots,” *Phys. Stat. Sol.* **224**, 727-734 (2001).
- 405.** E.P.A.M. Bakkers, Z. Hens, A. Zunger, A. Franceschetti, L.P. Kouwenhoven , L. Gurevich, D. Vanmaekelbergh, “Shell tunneling spectroscopy of the single-particle energy levels of insulating quantum dots,” *Nanoletters* **1**, 551-556 (2001).
- 406.** S. Muller, L.W. Wang and C. Wolverton, “Prediction of Alloy Precipitate Shapes from First-Principles,” *Europhysics Letters* **55**, 33-39 (2001).
- 407.** S. Muller, C. Wolverton, L.W. Wang and A. Zunger, “Predicting the Size and Temperature-Dependent Shapes of Precipitates in Al-Zn Alloys,” *Acta Materialia* **48**, 4007 (2000).
- 408.** S. Muller and A. Zunger, “The Structure of Ordered and Disordered α -Brass,” *Physical Review B* **63**, Article No.094204 (2001).

- 409.** S. Muller and A. Zunger, "First-Principles Prediction of Yet Unobserved Ordered Structures in the Ag-Pd Phase-Diagram," *Physical Review Letters* **87**, Article No. 165,502 (Oct. 2001).
- 410.** S. Muller, L.W. Wang and A. Zunger, "First-principles kinetic theory of precipitate evolution in Al-Zn alloys," *Modeling and Simulations in Material Science* **10**, 1-15 (2002).
- 411.** V. Ozolins and A. Zunger, "First-principles theory of the evolution of vibrational properties with long-range order in GaInP₂," *Phys. Review B* **63**, Article No.087202 (2001).
- 412.** A. Zunger, K. Kim and V. Ozolins, "Why are the conventionally-assumed high-pressure crystal structures of ordinary semiconductors unstable?" *Phys. Stat. Solidi B* **223**, 369-378 (2001).
- 413.** S.B. Zhang, S.H. Wei and A. Zunger, "p vs. n Doping Asymmetry and Defect Physics in ZnO," *Phys. Review B* **63**, Article No.075,205 (2001).
- 414.** K. Kim and A. Zunger, "Spatial correlations in GaInAsN alloys and their effects on band gap enhancement and electron localization," *Physical Review Letters* **86**, 2609-2612 (2001).
- 415.** P.R.C. Kent and A. Zunger, "Evolution of III-V nitride alloy electronic structure: the localized to delocalized transition," *Physical Review Letters* **86**, 2613-2616 (2001).
- 416.** P.R.C. Kent and A. Zunger, "Theory of Electronic Structure Evolution in GaAsN and GaPN Alloys," *Physical Review B* **64**, Article Number 115,208 (2001).
- 417.** P.R.C. Kent and A. Zunger, "Carrier localization and the origin of luminescence in cubic InGaN alloys," *Appl. Phys. Lett.* **79**, 1977 (2001).
- 418.** P.R.C. Kent and A. Zunger, "Nitrogen pairs and clusters in GaAs and GaP," *Appl Phy. Lett.* **79**, 2339 (2001).
- 419.** P.R.C. Kent and A. Zunger, "Evolution of electronic states with composition in GaAsN alloys," *Phys. Stat. Solidi.* **228B**, 253 (2001).
- 420.** A. Zunger, "Quantum Architecture of Novel Solids," *Annalen der Physik* **10**, 89-94 (2001).
- 421.** D. Regelman, E. Dekel, D. Gershoni, E. Ehrenfroind, A.J. Williamson, J. Shumway and A. Zunger, "Optical Spectroscopy of single quantum dots at a tunable positive, neutral, and negative charge states," *Physical Review B.* **64**, Article No. 165,301 (2001).
- 422.** R. Magri and A. Zunger, "Effects of interfacial atomic segregation on optical properties of InAs/GaSb superlattices," *Phys. Rev. B, Rapid Communications* **64**, 081305 (2001).

- 423. G.L. Hart and A. Zunger, "Origins of non-stoichiometry and vacancy ordering in ScS," *Physical Review Letters* **87**, Article No. 275,508 (Dec. 2001).
- 424. J.E. Jaffe and A. Zunger, "Defect-induced non-polar-to-polar transition at the surface of chalcopyrite semiconductors," *Phys. Rev., Rapid Communications* **64**, 241304 (2001).

2002 (425 - 437)

- 425. C. Kilic and A. Zunger, "Origins of co-existence of conductivity and transparency in SnO₂," *Physical Review Letters* **88**, Article No. 095501 (March 2002).
- 426. C. Kilic and A. Zunger, "n-type doping of oxides by hydrogen," *Appl. Physics Letters* **80**, 73 (2002).
- 427. P. Mahadevan and A. Zunger, "Origin of room temperature ferromagnetism in Mn doped semiconducting CdGeP₂," *Physical Review Letters* **88**, 047205 (28 Jan. 2002).
- 428. Alex Zunger, "On the Farsightedness (hyperopia) of the Standard k•p Model," *Phys. Stat. Solidi* **190(a)**, 467-475 (2002).
- 429. A. Zunger, "Unusual Physics in III-V Alloys: Spontaneous Ordering and Wavefunction Localizations," in "Physics of Semiconductors 2002," Institute of Physics Conf. Sec. 171, edt. R. Long and J.H. Davis, Bristol, U.K., p.47 (2002).
- 430. R. Magri and Alex Zunger, "Effects of Interfacial Atomic Segregation and Intermixing on the Electronic Properties of InAs/GaSb Superlattices," *Physical Review B* **65**, 165302 (2002).
- 431. R. Magri and A. Zunger, "Segregation Effects on the Optical Properties of InAs/GaSb Superlattices," *Physica E* **13**, 325 (2002).
- 432. K. Kim, G.L. Hart and A. Zunger, "Negative Band Gap Bowing in Epitaxial InAs/GaAs Alloys and Predicted Band Offsets of the Strained Binaries and Alloys on Various Substrates," *Applied Physics Letters* **80**, 3105 (2002).
- 433. K. Kim, P.R.C. Kent, A. Zunger and C. Gellar, "Atomistic Description of the Electronic Structure of InAs/GaAs Alloys and Superlattices," *Physical Review B*. **66**, 045208 (2002).
- 434. P.R.C. Kent, G. Hart and A. Zunger, "Biaxial Strain-Modified Valence and Conduction Band Offsets of Zincblende GaN, GaP, GaAs, InN, InP, InAs and Optical Bowing of Strained Epitaxial InGaN Alloys," *Applied Physics Letters* **81**, 4377 (2002).
- 435. P.R.C. Kent, L. Bellaiche and A. Zunger, "Pseudopotential Theory of III-V Nitrides," *Semiconductor Science & Technol.* **17**, 851-859 (2002).

- 436. L.G. Wang and A. Zunger, "Phosphorus and Sulphur Doping of Diamond," *Phys. Rev. B, Rapid Communications* **66**, 161202 (R) (2002).
- 437. A. Zunger, L.G. Wang, G. Hart and M. Sanati, "Obtaining Ising-like Expansions for Binary Alloys from First-Principles," *Modeling and Simulations in Material Science and Engineering* **10**, 685-706 (2002).

2003 (438 - 459)

- 438. L.G. Wang and A. Zunger, "Cluster Doping Approach for Wide-Gap Semiconductors," *Physical Review Letters* **90**, 256401 (2003).
- 439. L.G. Wang and A. Zunger, "Why are the 3d-5d Compounds CuAu and NiPt Stable, whereas the 3d-4d Compounds CuAg and NiPd Are Not?" *Physical Review B* **67**, 092103 (2003).
- 440. L.G. Wang and A. Zunger, "Dilute Non-isovalent (II-VI)-(III-V) Semiconductor Alloys: Monodoping, Co-doping and Cluster Doping in ZnSe-GaAs," *Phys. Rev. B* **68**, 125211 (2003).
- 441. M. Sanati, L.G. Wang and A. Zunger, "Adaptive Crystal Structures: CuAu and NiPt," *Physical Review Letters* **90**, 045502 (2003).
- 442. M. Sanati, G. Hart and A. Zunger, "Ordering Tendencies in Octahedral MgO-ZnO Alloys," *Phys. Rev. B* **68**, 155210 (2003).
- 443. C. Kilic and A. Zunger, "n-type Doping and Passivation of CuInSe₂ and CuGaSe₂ by Hydrogen," *Physical Review B* **68**, 075201 (2003).
- 444. C. Kilic and A. Zunger, "Doping of Chalcopyrites by Hydrogen," *Applied Physics Letters* **83**, 2007 (2003).
- 445. P.R.C. Kent and A. Zunger, "Failure of Nitride Levels to emerge from Gap with Pressure," *Appl. Phys. Letters* **82**, 559 (2003).
- 446. G. Bester, S. Nair and A. Zunger, "Pseudopotential Calculation of the Excitonic Fine-Structure of Million Atom Self-Assembled InGaAs/GaAs Quantum Dots," *Phys. Rev. B, Rapid Communications* **67**, 161306 (2003).
- 447. G. Bester and A. Zunger, "Compositional and Size-Dependent Spectroscopic Shifts due to Charged Excitons in Self-Assembled InGaAs/GaAs Quantum Dots," *Physical Review B* **68**, 073309 (2003).

- 448.** A. Zunger and G. Bester, "Theory of Excitons, Charged-Excitons, Exciton Fine-Structure and Entangled Excitons in Self-Assembled Semiconductor Quantum-Dots," *Physica E* **21**, 204-210 (2004).
- 449.** M. Califano, G. Bester and A. Zunger, "Prediction of a Shape-Induced Enhancement in the Hole Relaxation in Nanocrystals," *Nanoletters* **3**, 1197-1202 (2003).
- 450.** L.W. Wang, M. Califano, A. Zunger and A. Franceschetti, "Pseudopotential Theory of Auger Processes in CdSe Quantum Dots," *Physical Review Letters* **91**, 056404 (2003).
- 451.** C. Person and A. Zunger, "Deep Nitrogen-Induced Valence and Conduction Band States in GaAsN," *Phys. Review B* **68**, 035212 (2003).
- 452.** C. Person and A. Zunger, "s-d Coupling in Zincblende Semiconductors," *Physical Review B* **68**, 073205 (2003).
- 453.** C. Person and A. Zunger, "Anomalous Grain Boundary Physics in Polycrystalline CuInSe₂: The Existence of Hole Barrier," *Physical Review Letters* **91**, 266401 (2003).
- 454.** A. Zunger, "Practical Doping Rules," *App. Phys. Letters* **83**, 57 (2003).
- 455.** S. Dudiy and A. Zunger, "Optical Consequences of Long Range Order in Wurtzite AlGaN Alloys," *Physical Review B, Rapid Communications* **68**, 041302 (2003).
- 456.** P. Mahadevan and A. Zunger, "Ferromagnetism in Mn-doped GaAs due to Substitutional-Interstitial Complexes," *Physical Review B* **68**, 075202 (2003).
- 457.** R. Magri and A. Zunger, "Predicting Interband Transition Energies for InAs/GaSb Superlattices using the Empirical Pseudopotential Method," *Phys. Review B* **68**, 155329 (2003).
- 458.** R. Magri and A. Zunger, "Theory of Optical Properties of 6.1 Δ III-V Superlattices: The Role of the Interface," *J. Vac. Sci. Technol. B* **21**, 1896 (2003).
- 459.** R. Magri and A. Zunger, "Theory of Optical Properties of Segregated InAs/GaSb Superlattices," *IEE Proceedings Optoelectronics* **140**, 409 (2003).

2004 (460 - 476)

- 460.** G. Bester, J. Shumway and Alex Zunger, "Theory of Excitonic Spectra and Entanglement in Dot Molecules," *Physical Review Letters* **93**, 047401 (2004).

461. L. He, G. Bester and A. Zunger, “Strain-induced interfacial hole-localization in self-assembled quantum dots: compressive InAs/GaAs vs. tensile InAs/InSb,” *Physical Review B* **70**, 235316 (2004).
462. V. Blum and A. Zunger, “Structural Complexity in Binary bcc Ground States – the case of bcc Mo-Ta,” *Physical Review B, Rapid Communications* **69**, 02010 (2004).
463. V. Blum and A. Zunger, “Mixed-Basis Cluster Expansion for Thermodynamics of bcc Alloys,” *Phys. Review B* **70**, 155108 (2004).
464. P. Mahadevan and A. Zunger, “First-Principles Investigation of the Assumption Ferromagnetism of 3d Transition Metal Impurities in GaAs,” *Physical Review B* **69**, 115211 (2004).
465. P. Mahadevan and A. Zunger, “Trends in Ferromagnetism, Hole Localization and Acceptor Level Depth for Mn in GaN, GaP, GaAs, GaSb,” *App. Phys. Letters* **85**, 2860 (2004).
466. P. Mahadevan and A. Zunger, “Unusual Directional Dependence of Exchange Energies in GaAs: Mn, is the RKKY limit ever relevant?” *Physical Review Letters* **93**, 177201 (2004).
467. M. Califano, A. Franceschetti and A. Zunger, “Efficient Inverse Auger Recombination at Threshold in CdSe Nanocrystals,” *Nanoletters* **4**, 525-531 (2004).
468. M. Califano, A. Franceschetti and A. Zunger, “Direct Carrier Multiplication due to Inverse Auger Scattering in CdSe Quantum Dots,” *Appl. Phys. Letters* **84**, 2409 (2004).
469. M. Califano and A. Zunger, “Anisotropy of Interband Transitions in InAs Quantum Wires,” *Phys. Rev. B* **70**, 165317 (2004).
470. Y.J. Zhao and A. Zunger, “Site Preference for Mn Substitution in Spintronic CuMnX₂ Chalcopyrite Semiconductors,” *Phys. Rev. B* **69**, 075208 (2004).
471. Y.J. Zhao and A. Zunger, “Electronic Structure and Ferromagnetism of Mn-Substituted CuAlS₂, CuGaS₂, CuInS₂, CuGaTe₂, *Phys. Rev. B* **69**, 104422 (2004).
472. Y.J. Zhao, P. Mahadevan and A. Zunger, “Comparison of predicted ferromagnetic tendencies of Mn substituting the Ga site in III-V’s and in I-III-VI₂ chalcopyrite semiconductors,” *App. Phys. Letters* **84**, 3753 (2004).
473. Y.J. Zhao, C. Persson, S. Lany and A. Zunger, “Why can CuInSe₂ be readily equilibrium doped n-type, but the wider-gap CuGaSe₂ cannot?” *Appl. Phys. Lett.* **85**, 5860 (2004).
474. S.V. Dudy and A. Zunger, “Type-I to Type-II Transition at the Interface Between Random and Ordered Domains of AlGaN,” *Appl. Phys. Lett.* **84**, 1874 (2004).

- 475. S.V. Dudy, P. Kent and A. Zunger, “Penetration of electronic perturbations of dilute nitrogen impurities deep into the conduction band of GaPN,” *Physical Review B Rapid Communication* **70**, 161304 (2004).
- 476. S. Lany and A. Zunger, “Metal-Dimer Atomic Reconstruction leading to deep donor states in anion vacancy in II-VI and chalcopyrite semiconductors,” *Physical Review Letters* **93**, 156404 (2004).

2005 (477 - 501)

- 477. S. Lany, Y.J. Zhao, C. Persson and A. Zunger, “Halogen n-type doping of chalcopyrite semiconductors,” *Appl. Physics Letters* **86**, 042109 (2005).
- 478. S. Lany and A. Zunger, “Anion vacancies as a source of persistent photoconductivity in II-VI and chalcopyrite semiconductors,” *Physical Review B* **72**, 035215 (2005).
- 479. S. Lany and A. Zunger, “Light and Bias-induced Metastability in Cu(In, Ga)Se caused by Vse-Vcu Vacancy Complex,” submitted to *Physical Review B*.
- 480. C. Persson, Y.J. Zhao, S. Lany and A. Zunger, “n-type doping of CuInSe₂ and CuGaSe₂,” *Physical Review B* **72**, 035211 (2005).
- 481. C. Persson and A. Zunger, “A Compositionally-Induced Valence Band Offset at the Grain Boundaries of Polycrystalline Chalcopyrites Creates a Hole Barrier,” *Applied Physics Letters* **87**, 211,904 (2005).
- 482. M.J. Hetzer, Y.M. Strzhemechny, M. Gao, L.J. Brillson, M. Contreras and A. Zunger, “Direct observation of copper depletion and potential changes at CuInGaSe₂ grain boundaries,” *Applied Physics Letters* **86**, xxx (2005).
- 483. P. Mahadevan, J.M. Osorio-Guillen and A. Zunger, “Origin of Transition Metal Clustering Tendencies in GaAs – Based Dilute Magnetic Semiconductors,” *Applied Physics Letters* **86**, 172,504 (2005).
- 484. Y.J. Zhao and A. Zunger, “Practical Rules for Orbital-Controlled Ferromagnetism of 3d Impurities in Semiconductors,” *Journal of Applied Physics* **98**, 113,901 (2005).
- 485. Y.J. Zhao and A. Zunger, “Zincblende Half-Metallic Ferromagnets are Rarely Stabilized by Epitaxy,” *Physical Review B* **71**, 132,403 (2005).
- 486. G. Bester, J. Shumway and A. Zunger, “Broken Symmetry and Quantum Entanglement of an Exciton in InAs/GaAs Quantum Dot Molecules,” *Physical Review B* **71**, 075325 (2005).

487. G. Bester and A. Zunger, "Cylindrically Shaped Zincblende Semiconductor Quantum Dots Do Not Have Cylindrical Symmetry: Atomistic Symmetry, Atomic Relaxation and Piezoelectric Effects," *Physical Review B* **71**, 045318 (2005).
488. G. Bester and A. Zunger, "Electric Field Control and Optical Signature of Entanglement in Quantum Dot Molecules," *Physical Review B* **72**, 165,334 (2005).
489. L. He, G. Bester and A. Zunger, "Prediction of an Excitonic Ground State in InAs/InSb Quantum Dots," *Physical Review Letters* **94**, 016801-01 (2005).
490. L. He, G. Bester and A. Zunger, "Electronic Asymmetry in Self-Assembled Quantum Dot Molecules Made of Identical InAs/GaAs Quantum Dots," *Physical Review B, Rapid Communications* **72**, 081,311 (2005).
491. L. He, G. Bester and A. Zunger, "Singlet-Triplet Splitting Correlation and Entanglement for two electrons in dot molecules," *Physical Review B* **72**, 195,307 (2005).
492. L. He, G. Bester and A. Zunger, "Electronic Phase Diagrams of Carriers in Self-Assembled InAs/GaAs Quantum Dots: Violation of Hund's Rule and the Aufbau Principle for Holes," *Physical Review Letters* **95**, 246,804 (2005).
493. L. He and A. Zunger, "Multiple Charging of InAs/GaAs Quantum Dots by Electrons or Holes: Addition Energies and Ground State Configurations," *Physical Review B* **73**, 115,324 (2006).
494. G.A. Narvaez, G. Bester and A. Zunger, "Pressure Effects on Neutral and Charged Excitons in Self-Assembled (InGa)As/GaAs Quantum Dots," *Phys. Rev. B Rapid Communications* **72**, 041307 (2005).
495. G.A. Narvaez, G. Bester and A. Zunger, "Excitons, Biexcitons and Trions in Self-Assembled InGaAs/GaAs Quantum Dots: Recombination Energies, Polarization and Radiative Lifetimes vs. Dot Height," *Physical Review B* **72**, 245,318 (2005).
496. G.A. Narvaez, G. Bester and A. Zunger, "Dependence of the Electronic Structure of Self-Assembled InGaAs/GaAs Quantum Dots on Height and Composition," *Journal of Applied Physics* **98**, 043,708 (2005).
497. R. Magri, A. Zunger and H. Kroemer, "Evolution of the band gap and band edge energies of the lattice-matched GaInAsSb/GaSb and GaInAsSb/InAs alloys as a function of composition," *Journal of Applied Physics* **98**, 043,701 (2005).
498. V. Blum and A. Zunger, "Prediction of ordered structures in bcc binary systems Mo, Nb, Ta and W from first-principles search of ~3,000,000 possible configurations," submitted to *Physical Review B Rapid Communications* **72**, 020104 (2005).

499. G. Hart, V. Blum, M. Walorski and A. Zunger, "Genetic determination of first-principles Hamiltonians," *Nature Materials* **4**, 391 (2005).
500. V. Blum, G. Hart, M.J. Walorski and A. Zunger, "Using Genetic Algorithms to Map First-Principles Results to Model Hamiltonians," *Physical Review B* **72**, 165,113 (2005).
501. M. Califano, A. Franceschetti and A. Zunger, "Temperature-Dependence of Excitonic Radiative Decay in CdSe Quantum Dots: The Role of Surface Hole Traps," *Nanoletters* **5**, 2360 (2005).

2006 (502 -)

502. S.V. Dudiy and A. Zunger, "Searching for Alloy Configurations with Extreme Physical Properties: Genetic Algorithm Inverse Band Structure of Ga(P, N)," *Physical Review Letters* **97**, 046401 (2006).
503. S.V. Dudiy, A. Zunger, M. Felici, A. Polimeni, M. Capizzi, H.P. Xin and C.W. Tu, "Nitrogen-Induced Perturbation of the Valence Band States in Ga(P, N) Alloys," *Physical Review B* **74**, 155,303(2006)
504. A. Franceschetti, S.V. Barabash, J. Osorio, A. Zunger and M. Van Schilfgaarde, "Enhancement of Interactions Between Magnetic Ions in Semiconductors Due to De-Clustering," *Phys. Rev. B Rapid Communication* (In Press).
505. A. Franceschetti, L.W. Wang, G. Bester and A. Zunger, "Confinement-Induced vs. Correlation-Induced Electron Localization in Model Semiconductor Nano Circuits," *Nanoletters* **6**, 1069 (2006).
506. S.V. Barabash, V. Blum, S. Muller and A. Zunger, "Prediction of Unusual Stable Ordered Structures of Au-Pd Alloys Via a First-Principles Cluster Expansion," *Physical Review B* **74**, 035108 (2006).
507. J. Osorio-Guillen, Y.J. Zhao, S.V. Barabash and A. Zunger, "Structural Stability of (Ga, Mn) as Random Alloys, Ordered Compounds and GaAs/MnAs Superlattices from First-Principles," *Physical Review B* **74**, 035305 (2006).
508. J.M. Osorio, S. Barabash, S. Lany and Alex Zunger, "Magnetism Without Magnetic Ions: Percolation, Exchange and Formation Energies of Magnetism-Promoting Intrinsic Vacancies in CaO," *Physical Review Letters* **96**, 107203 (2006).
509. J. An, A. Franceschetti, S. Dudiy and A. Zunger, "The Peculiar Electronic Structure of PbSe," *Nanoletters* (In Press).

- 510.** A. Franceschetti, S. Dudiy, S. Barabash, A. Zunger and M. vanSchifffgaarde, “First-Principles Combinatorial Design of Transition Temperature in Multicomponent Systems,” *Physical Review Letters* **97**, 047202 (2006).
- 511.** G. Narvaez and A. Zunger, “Nominally-Forbidden Interband Optical Transitions in Quantum Dots,” *Physical Review B* **74**, 045316 (2006)
- 512.** A. Franceschetti, J. An and A. Zunger, “Impact Ionization Can Explain Carrier Multiplication in PbSe Quantum Dots,” *Nanoletters* **6**, 2191 (2006).
- 513.** G. Bester, A. Zunger, X. Wu and D. Vanderbilt, “Importance of Piezoelectric Properties of InAs/GaAs Quantum Dots,” *Physical Review Letters* **96**, 187602 (2006).
- 514.** G. Bester, A. Zunger, X. Wu and D. Vanderbilt, “The Nonlinear Peizoelectric Effect,” *Physical Review B Rapid Communication* **74**, 081305 (2006).
- 515.** G. Narvaez, G. Bester, and A. Zunger, “Carrier Relaxation Mechanisms in Self-Assembled (In,Ga)As/GaAs Quantum Dots: Efficient P-> S Auger Relaxation of Electrons,” *Physical Review B* **74**, 075403 (2006).
- 516.** M.J. Hetzer, Y.M. Strzhemechny, M. Gao, and A. Zunger, “On Microscopic Compositional and Electrostatic Properties of Grain Boundaries in Polycrystalline CuIn_{1-x}Ga_xSe₂,” *Journal of Vacuum Science & Technology B* **24**, 1739-1745 (2006).
- 517.** G. Trimarchi, P. Graf, and A. Zunger, “Exploring the Configurational Space of Binary Alloys: Different Sampling for Different Cell Shapes,” *Physical Review B* **74**, 014204 (2006).
- 518.** G. A. Narvaez, L.X. He, G. Bester, and A. Zunger, “Theoretical Predictions of the Electronic and Optical Properties of Single and Coupled (In,Ga)As/GaAs Quantum Dots,” *Physica E-Low-Dimensional Systems & Nanostructures* **32**, 93-96 (2006).
- 519.** G.A. Narvaez and A. Zunger, “Calculation of Conduction-to-Conduction and Valence-to-Valence Transitions Between Bound States in (In,Ga)As/GaAs Quantum Dots,” *Phys. Rev. B*.
- 520.** G.A. Narvaez, G. Bester, A. Franceschetti, and A. Zunger, “Excitonic Exchange Effects on the Radiative Decay Time of Monoexcitons and Biexcitons in Quantum Dots,” *Phys. Rev. B* **74**, 205422 (2006)
- 521.** L. He and A. Zunger, “Electronic Structures of (In,Ga)As/GaAs Quantum Dot Molecules Made of Dots with Dissimilar Sizes,” *Phys. Rev. B* (In Press).
- 522.** A. Zunger, A. Franceschetti, G. Bester, W.B. Jones, K. Kim, P.A. Graf, L.-W. Wang, A. Canning, O. Marques, C. Voemel, J. Dongarra, J. Langou, and S. Tomov, “Predicting the

Electronic Properties of 3D, Million-Atom Semiconductor Nanostructure Architectures,” *J. of Physics*, **46** (2006) 292-298.

523. M. Ediger, G. Bester, B. D. Gerardot, A. Badolato, P.M. Petroff, K. Karrai, A. Zunger, and R.J. Warburton, “Fine Structure of Negatively and Positively Charged Excitons in Semiconductor Quantum Dots: Electron-Hole Asymmetry,”
524. M. Ediger, G. Bester, A. Badolato, P.M. Petroff, K. Karrai, A. Zunger, and R. J. Warburton, “Peculiar Many-Body Effects Revealed in the Spectroscopy of Heavily Charged Quantum Dots,”
525. S. Barthlein, E. Winning, G.L.W. Hart, A. Zunger, and S. Muller, “Long-Period Superstructures in Binary Alloys: Predicted Stability of 1D- and Instability of 2D-Superstructures,”
526. S. Barthlein, G.L.W. Hart, A. Zunger, and S. Muller, “Reinterpreting the Cu-Pd Phase Diagram Based on New-Ground-State Predictions,”
527. S. Lany and A. Zunger, “Light and Bias Induced Metastability in Cu(In,Ga)Se₂ Based Solar cells Caused by the (V_{Sc}-V_{Cu}) Vacancy Complex,” *J. Appl. Phys.*
528. G. Trimarchi and A. Zunger, “The Global Space-Group Optimization Approach to Finding the Stablest Crystal Structure,”
529. M. Califano, A. Franceschetti and A. Zunger, “Lifetime and Polarization of the Radiative Decay of Excitons, Biexcitons and Trions in CdSe Nanocrystal Quantum Dots,”

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