Su-Huai Wei

Work Address:
National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, Colorado 80401-3393
PH: 303-384-6666; FAX: 303-384-6432; e-mail: swei@nrel.gov

EDUCATION

8/85 Ph.D. in Physics, College of William and Mary in Virginia.
Thesis: First-Principles Structure Calculations Using the General Potential LAPW Method
Advisor: Professor Henry Krakauer

5/83 M.S. in Physics, College of William and Mary in Virginia.

6/81 B.S. in Physics, Fudan University, Shanghai, China.

WORK EXPERIENCE

10/06 to present
Principal Scientist and Group Manager, Theoretical Materials Science
National Renewable Energy Laboratory (NREL) (formerly SERI).

4/03 to 9/06
Principal Scientist (since 04/03) and Team Leader, Computational Materials Science, NREL.

4/95 to 3/03
Senior Scientist II and Team Leader (since 10/99), NREL.

4/92 to 3/95
Senior Scientist I, NREL.

1/90 to 3/92
Staff Scientist, NREL.

8/85 to 12/89
Postdoctoral Researcher/Research Associate, Solar Energy Research Institute (SERI).

8/81 to 8/85
Graduate Teaching/Research Assistant, College of William and Mary.
Research Subject: Muon spin resonance; Electronic structure theory.

12/75 to 2/78
Mathematics Teacher, Technical School Affiliated to Shanghai Plastics Research Institute.

AREAS OF SPECIALIZATION

Research Interests

My Current research is focused on developing first-principles electronic structure theory of solids, which includes studying (i) electronic structures and stabilities of alloys, superlattices. and interfaces; (ii) magnetic properties of semiconductors; (iii) optoelectronic properties of photovoltaic and light-emitting materials; (iv) electronic properties of organic and hybrid semiconductors (v) defect physics in semiconductors and nanocrystals; and (vi) hydrogen storage materials.

Scientific Achievements

Developed a completely general, full potential, self-consistent LAPW code for electronic structure and total energy calculations. Made original and significant contributions to the understanding of (i) electronic structures and stabilities of semiconductor and metallic alloys, superlattices, surfaces, and filled-tetrahedron compounds; (ii) effect of d and f electrons in II-VI and magnetic semiconductors; (iii) chemical trends of band offsets and pressure coefficients of semiconductors; (iv) electronic structures of wide band gap nitrides and oxides; (v) defect physics in semiconductors and nanocrystals; and (vi) electronic structure of nano, organic, and hybrid semiconductors.

Languages:

Fluent in English and Chinese.

Publications and Presentations:

More than 250 peer-reviewed publications, including 58 papers in the prestigious **Physical Review Letters** and **Physical Review Rapid Communications**, and more than 7900 citations (H factor: 48). Presented many invited talks in international conferences.

Some of the recent invited talks are:

"First Principles Design of Functional Materials",The Third International Workshop on DFT applied to Metals and Alloys", May 2-4, 2007, Oran Algeria

"Overcoming the doping limit in wide gap semiconductors", The XXXVI International School on the Physics of Semiconducting compounds", June 9-15, 2007, Jaszowiec, Poland.

"Band coupling model of ferromagnetism in Semiconductors" The SPIE Photoniic West (OPTO2008), January 20-24, 2008,

Professional Membership:

American Physical Society, Materials Research Society

HONORS AND AWARDS

Chunky Bullet Award, DOE/BES 2002
Outstanding Performance Award, NREL, 2001
Fellow of American Physical Society, 1999
Outstanding Researcher Award, DOE, 1995
Graduate Student Fellowship, College of William and Mary, 1981 - 1985
Winner of the CUSPEA (China-U.S. Physics Education and Application), 1981

PUBLICATIONS

Numbers in [ ] is the citation number according to ISI on September 1, 2006

(1) "Zero field muon spin depolarization revisited", K. G. Petzinger and **S.-H.Wei**, Hyperfine Interaction **17-19**, 441 (1984).[1]

(2) "Local-density-functional calculation of the pressure-induced metalization of BaSe and BaTe", **S.-H. Wei** and H. Krakauer, **Phys Rev. Lett. 55**, 1200 (1985).[380]

(3) "Linearized augmented-plane wave calculation of the electronic structure and total energy of tungsten", **S.-H. Wei**, H. Krakauer, and M. Weinert, Phys. Rev. B **32**, 7792 (1985).[96]

(4) "Instability of the ideal tungsten (001) surface", D. Singh, **S.-H. Wei**, and H. Krakauer, **Phys. Rev. Lett. 57**, 3292 (1986).[43]

(5) "Electronic structure and phase stability of LiZnAs: A half ionic and half covalent tetrahedral semiconductor", **S.-H. Wei** and A. Zunger, **Phys. Rev. Lett. 56**, 528 (1986).[31]

(6) "Alloy-stabilized semiconducting and magnetic zinc-blende phase of MnTe", **S.-H. Wei** and A. Zunger, **Phys. Rev. Lett. 56**, 2391 (1986).[55]

(7) "Thermodynamic instability of ultrathin semiconductor superlattices", D.M. Wood, **S.-H. Wei**, and A. Zunger, **Phys. Rev. Lett. 58**, 1123 (1987).[50]

(8) "Total energy and band structure calculation for the semimagnetic $Cd_{1-x}Mn_xTe$ semiconductor alloy and its binary constituents", **S.-H. Wei** and A. Zunger, Phys. Rev. B **35**, 2340 (1987).[161]

(9) "Phase stability and band structure of the semimagnetic $Cd_{1-x}Mn_xTe$ semiconductor alloy", **S.-H. Wei** and A. Zunger, in *Ternary and Multinary Compounds*, edited by S. K. Deb and A. Zunger, (Material Research Society, Pittsburgh, 1987), p.485.

(10) "Electronic structure and stability of $A^{I}B^{II}C^{V}$ filled tetrahedral compounds", D. M. Wood, **S.-H. Wei**, and A. Zunger, in *Ternary and Multinary Compounds*, edited by S. K. Deb and A. Zunger, (Material Research Society, Pittsburgh, 1987), p. 523.

(11) "Band structure and electronic excitations in $Cd_{1-x}Mn_xTe$", **S.-H. Wei** and A. Zunger, in *Diluted Magnetic (Semimagnetic) Semiconductors*, edited by J. K. Furdyna, R. L. Aggarwal, and S. von Molnar (Material Research Society, Pittsburgh, 1987), p. 197 (1987).

(12) "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", D. G. Kilday, G. Margaritondo, T. F. Ciszek, S. K. Deb, **S.-H. Wei** and A. Zunger, Phys. Rev. B **36 (Rapid Communication)**, 9388 (1987).[9]

(13) "Electronic structure of M^{I}_3Sb-type filled tetrahedral semiconductors", **S.-H. Wei** and A. Zunger, Phys. Rev. B **35**, 3952 (1987).[5]

(14) "Role of *d* orbital in valence band offsets of common-anion semiconductors", **S.-H. Wei**, and A. Zunger, **Phys. Rev. Lett. 59**, 144 (1987).[123]

(15) "Comment on 'Coulomb energy in pseudobinary alloys' ", **S.-H. Wei**, **Phys. Rev. Lett. 59**, 2613 (1987).[7]

(16) "Calculation of the valence band offsets of common-anion semiconductor heterojunctions from core levels: the role of cation *d* orbital", **S.-H. Wei** and A. Zunger, J. Vac. Sci. & Technol. B **5**, 1239 (1987).[16]

(17) "First-principles calculations of the phase diagrams of noble metals: Cu-Au, Cu-Ag and Ag-Au", **S.-H. Wei**, A. A. Mbaye, L. G. Ferreira, and A. Zunger, Phys. Rev. B **36**, 4163 (1987).[80]

(18) "The solution of large dense generalized eigenvalue problems on the Cray X-MP/24 with SSD", G. Roger, H. Krakauer, J. Lewis, H. Simon, and **S.-H. Wei**, J. Comput. Phys. **69**, 471 (1987).[3]

(19) "Stability and electronic structure of ultrathin [001] $(GaAs)_m(AlAs)_m$ superlattices", D. M. Wood, **S.-H. Wei**, and A. Zunger, Phys. Rev. B **37**, 1342 (1988).[50]

(20) "Ordering-induced changes in the optical spectra of semiconductor alloys", J. E. Bernard, **S.-H. Wei**, D. M. Wood, and A. Zunger, Appl. Phys. Lett. **52**, 311 (1988).[28]

(21) "A novel viewpoint on the Cu-Au phase diagram: the interplay between fixed Ising energies and elastic effects", A. Zunger, **S.-H. Wei**, A. A. Mbaye, and L. G. Ferreira, Acta Metall. **36**, 2239 (1988).[18]

(22) "Electronic structure of II-VI compounds and their alloys: role of cation d bands", **S.-H. Wei** and A. Zunger, J. Crystal Growth **86**, 1 (1988).[8]

(23) "Role of metal d states in II-VI semiconductors", **S.-H. Wei** and A. Zunger, Phys. Rev. B **37**, 8958 (1988).[197]

(24) "Electronic structure of ultrathin $(GaAs)_n(AlAs)_n$ [001] superlattices and the $Ga_{0.5}Al_{0.5}As$ alloy", **S.-H. Wei**, and A. Zunger, J. Appl. Phys. **63**, 5794 (1988).[63]

(25) "Electronic structure and stability of II-VI semiconductors and their alloys: the role of metal *d* bands", **S.-H. Wei** and A. Zunger, J. Vac. Sci. & Technol. A **6**, 2597 (1988).[43]

(26) "Ordering of isovalent intersemiconductor alloys", J. E. Bernard, L. G. Ferreira, **S.-H. Wei**, and A. Zunger, Phys. Rev. B **38 (Rapid Communication)**, 6338 (1988).[67]

(27) "Thermodynamic stability of $(AlAs)_n(GaAs)_n$ superlattices and the random $Al_{0.5}Ga_{0.5}As$ alloy", **S.-H. Wei** and A. Zunger, **Phys. Rev. Lett. 61**, 1505 (1988).[30]

(28) "(111)-oriented $(GaAs)_n(AlAs)_n$ superlattices are direct band-gap materials for all n's" **S.-H. Wei** and A. Zunger, Appl. Phys. Lett. **53**, 2077 (1988).[20]

(29) "Epitaxy-induced structural phase transformations", S. Froyen, **S.-H. Wei**, and A. Zunger, Phys. Rev. B **38 (Rapid Communication)**, 10124 (1988).[46]

(30) "First-principles calculation of alloy phase diagrams: the renormalized interaction approach", L. G. Ferreira, **S.-H. Wei**, and A. Zunger, Phys. Rev. B **40**, 3197 (1989).[112]

(31) "Band gaps and spin-orbit splitting of ordered and disordered $Al_{1-x}Ga_xAs$ and $GaAs_xSb_{1-x}$ alloys", **S.-H. Wei** and A. Zunger, Phys. Rev. B **39**, 3279 (1989).[160]

(32) "Negative spin-orbit bowing in semiconductors alloys", **S.-H. Wei** and A. Zunger, Phys. Rev. B **39 (Rapid Communication)**, 6279 (1989).[14]

(33) "First-principles calculation of the formation energies of ordered and disordered phases of AlAs-GaAs", N. E. Christensen, **S.-H. Wei**, and A. Zunger, Phys. Rev. B **40**, 1642 (1989).[12]

(34) "First-principles theory of alloy phase diagram", A. Zunger, L. G. Ferreira, and **S.-H. Wei**, in *Atomic Scale Calculations in Material Science*, edited by J. Tersoff, D. Vanderbilt, and V. Vitek, (Material Research Society, Pittsburgh, 1989), p. 177.

(35) "Instability of diatomic deuterium in fcc palladium", **S.-H. Wei** and A. Zunger, J. Fusion Energy **9**, 367 (1990).[2]

(36) "Absence of volume metastability in bcc copper", Z. W. Lu, **S.-H. Wei**, and A. Zunger, Phys. Rev. B **41**, 2699 (1990).[25]

(37) "Stability of coherently strained semiconductor superlattices", R. G. Dandrea, J. E. Bernard, **S.-H. Wei**, and A. Zunger, **Phys. Rev. Lett. 64**, 36 (1990).[57]

(38) "Band gap narrowing in ordered and disordered semiconductor alloys", **S.-H. Wei** and A. Zunger, Appl. Phys. Lett. **56**, 662 (1990).[180]

(39) "Stability of atomic and diatomic hydrogen in fcc palladium", **S.-H. Wei** and A. Zunger, Solid State Commun. **73**, 327 (1990).[5]

(40) "First-principles calculation of temperature-composition phase diagrams of semiconductor alloys", **S.-H. Wei**, L. G. Ferreira, and A. Zunger, Phys. Rev. B. **41**, 8240 (1990).[132]

(41) "Special quasirandom structure", A. Zunger, **S.-H. Wei**, L. G. Ferreira, and J. E. Bernard, **Phys. Rev. Lett. 65**, 353 (1990).[166]

(42) "Ordering in semiconductor alloys", J. E. Bernard, R. G. Dandrea, L. G. Ferreira, S. Froyen, **S.-H. Wei**, and A. Zunger, Appl. Phys. Lett. **56**, 731 (1990).[30]

(43) "Electronic properties of random alloys: special quasirandom structures", **S.-H. Wei**, L. G. Ferreira, J. E. Bernard, and A. Zunger, Phys. Rev. B **42**, 9622 (1990).[116]

(44) "Ground state structures and the random state energy of the Madelung lattice", R. Magri, **S.-H. Wei**, and A. Zunger, Phys. Rev. B **42 (Rapid Communication)**, 11388 (1990).[82]

(45) "Stability, electronic structure and phase diagrams of novel inter-semiconductor compounds", L. G. Ferreira, **S.-H. Wei**, and A. Zunger, Inter. J. Supercomp. Appl. **5**, 34 (1991).[34]

(46) "Pseudopotential plane-wave calculations for ZnS", J. L. Martins, N. Troullier, and **S.-H. Wei**, Phys. Rev. B. **43**, 2213 (1991).[83]

(47) "Ground state structures of intermetallic compounds: a first-principles Ising model", Z. W. Lu, **S.-H. Wei**, and A. Zunger, Solid State Commun **78**, 583 (1991).[14]

(48) "First-principles statistical mechanics of structural stability of intermetallic compounds", Z. W. Lu, **S.-H Wei**, A. Zunger, S. Frota-Pessoa, and L. G. Ferreira, Phys. Rev. B **44**, 512 (1991).[166]

(49) "Disorder effects on the density of states of the II-VI semiconductor alloys $Hg_{0.5}Cd_{0.5}Te$, $Cd_{0.5}Zn_{0.5}Te$ and $Hg_{0.5}Zn_{0.5}Te$", **S.-H. Wei** and A. Zunger, Phys. Rev. B **43**, 1662 (1991); *ibid*, 14272 (1991).[62]

(50) "Long-range order in binary late transition metal alloys", Z. W. Lu, **S.-H. Wei**, and A. Zunger, **Phys. Rev. Lett. 66**, 1753 (1991).[57]

(51) "Electronic structure of random $Ag_{0.5}Pd_{0.5}$ and $Ag_{0.5}Au_{0.5}$ alloys", Z. W. Lu, **S.-H. Wei**, and A. Zunger, Phys. Rev. B **44**, 10470 (1991).[47]

(52) "Proposal for new III-V structures with infrared band gaps", **S.-H. Wei** and A. Zunger, Appl. Phys. Lett. **58**, 2684 (1991).[43]

(53) "Large lattice-relaxation-induced electronic level shifts in random $Cu_{1-x}Pd_x$ alloys", Z. W. Lu, **S.-H. Wei**, and A. Zunger, Phys. Rev. B **44 (Rapid Communication)**, 3387 (1991).[35]

(54) "Comment on origins of compositional order in NiPt alloys", Z. W. Lu, **S.-H. Wei**, and A. Zunger, **Phys. Rev. Lett. 68**, 1961 (1992).[19]

(55) "Electronic structures of ordered and disordered Cu_3Au and Cu_3Pd", Z. W. Lu, **S.-H. Wei**, and A. Zunger, Phys. Rev. B **45**, 10314 (1992).[60]

(56) "First-principles calculation of order-disorder transition in chalcopyrite semiconductors", **S.-H. Wei**, L. G. Ferreira and A. Zunger, Phys. Rev. B **45 (Rapid Communication)**, 2533 (1992).[42]

(57) "Theory of bonding charge density in β-NiAl", Z. W. Lu, **S.-H. Wei**, and A. Zunger, Acta Metall. Mater. **40**, 2155 (1992).[21]

(58) "Evolution of alloy properties with long-range order", D. B. Laks, **S.-H. Wei**, and A. Zunger, **Phys. Rev. Lett. 69**, 3766 (1992).[62]

(59) "Prediction of new low temperature structures using first-principles statistical mechanics", A. Zunger, Z. W. Lu, **S.-H Wei**, L. G. Ferreira, and S. Frota-Pessoa, in *Modern Topics of Condensed Matters*, edited by J. L. Heiras and T. Akachi (ETC, Morelos, Mexico, 1992), p. 147.

(60) "Stability and metastability of semiconductor alloys", L. G. Ferreira, A. Zunger, **S.-H. Wei**, Z. W. Lu, in *Semiconductor Physics*, edited by J. R. Leite, A. Fazzio, and A. S. Chaves, (World Scientific, Singapore, 1992), p. 42.

(61) "Relativity-induced ordering and phase-separation in intermetallic compounds", Z. W. Lu, **S.-H. Wei**, and A. Zunger, Euro. Phys. Lett. **21**, 221 (1993).[25]

(62) "First-principles phase diagrams of pseudoternary chalcopyrite/zinc-blende alloys" , R. Osorio, Z. W. Lu, **S.-H. Wei**, and A. Zunger, Phys. Rev. B **47 (Rapid Communication)**, 9985 (1993).[11]

(63) "Off-center atomic displacements in zinc-blende semiconductor", **S.-H. Wei**, S. B. Zhang, and A. Zunger, **Phys. Rev. Lett. 70**, 1639 (1993).[28]

(64) "Dependence of the optical properties of semiconductor alloys on the degree of long range order", **S.-H. Wei**, D. B. Laks, and A. Zunger, Appl. Phys. Lett. **62**, 1937 (1993); *ibid* **63**, 1292 (1993).[106]

(65) "Electronic origin of magnetic phase transition in zinc-blende Mn chalcogenides", **S.-H. Wei** and A. Zunger, Phys. Rev. B **48**, 6111 (1993).[27]

(66) "Electronic structure of II-VI semiconductor and their alloys", **S.-H. Wei**, in *II-VI Semiconductor Compounds*, edited by M. Jain (World Scientific, Singapore, 1993), p. 71.

(67) "Band offset at the $CdS/CuInSe_2$ heterojunction", **S.-H. Wei** and A. Zunger, Appl. Phys. Lett. **63**, 2549 (1993).[23]

(68) "Theoretical and experimental studies of the $ZnSe/CuInSe_2$ heterojunction band offset", A. J. Nelson, C. R. Schwerdtfeger, **S.-H. Wei**, A. Zunger, D. Rioux, R. Patel, and H. Hochst, Appl. Phys. Lett. **62**, 2557 (1993).[13]

(69) "Influence of Ga concentration on the ordering process of $Ga_xIn_{1-x}P$ grown on GaAs", A. Eyal, R. Beserman, **S.-H. Wei**, A. Zunger, E. Maayan, O. Kreinin, J. Salzman, R. Westphalen, and K. Heime, Jpn. J. Appl. Phys. Suppl. **32-3**, 716 (1993).[6]

(70) "Structural instability in zinc-blende semiconductors", **S.-H. Wei**, S. B. Zhang, and A. Zunger, Ferroelectrics, **155**, 127 (1994).[]

(71) "Prediction and observation of II-VI/$CuInSe_2$ heterojunction band offsets", A. J. Nelson, D. W. Niles, C. R. Schwerdtfeger, **S.-H. Wei**, A. Zunger, and H. Hochst, J. Electron Spectro. and Relat. Phenol. **68**, 185 (1994).[10]

(72) "Optical properties of zinc-blende semiconductor alloys: effects of epitaxial strain and chemical ordering", **S.-H. Wei** and A. Zunger, Phys. Rev. B. **49**, 14337 (1994).[88]

(73) "Strain effects on the spectra of spontaneously ordered $Ga_xIn_{1-x}P$", **S.-H. Wei** and A. Zunger, Appl. Phys. Lett. **64**, 757 (1994).[18]

(74) "Optical anisotropy and spin polarization in ordered GaInP", **S.-H. Wei** and A. Zunger, Appl. Phys. Lett. **64**, 1676 (1994).[24]

(75) "First principles simulated annealing study of phase-transition and short-range order in alloys", Z. W. Lu, D. B. Laks, **S.-H. Wei** and A. Zunger, Phys. Rev. B **50**, 6642 (1994).[47]

(76) "Relationships between the band gaps of the zinc-blende and wurtzite modifications of semiconductors", C.-Y. Yeh, **S.-H. Wei** and A. Zunger, Phys. Rev. B **50 (Rapid Communication)**, 2715 (1994).[35]

(77) "Type-II $\rightarrow$ type-I transition in $(GaX)_n/(InX)_n$ (001) superlattices (X=P, Sb) as a function of period n", A. Franceschetti, **S.-H. Wei**, and A. Zunger, Phys. Rev. B **50 (Rapid Communication)**, 8094 (1994).[10]

(78) "Absolute deformation potentials of Al, Si, and NaCl", A. Franceschetti, **S.-H. Wei**, and A. Zunger, Phys. Rev. B **50**, 17797 (1994).[14]

(79) "E_1, E_2, and E_0' transitions and pressure dependence in ordered $Ga_{0.5}In_{0.5}P$", **S.-H. Wei**, A. Franceschetti, and A. Zunger, Phys. Rev. B **51**, 13097 (1995).[13]

(80) "Theory of reflectance difference spectroscopy in ordered III-V semiconductor alloys", **S.-H. Wei** and A. Zunger, Phys. Rev. B **51**, 14110 (1995).[10]

(81) "Band offset and optical bowing of chalcopyrite and Zn-based II-VI alloys", **S.-H. Wei** and A. Zunger, J. Appl. Phys. **78**, 3846 (1995).[79]

(82) "Optical properties of $Ga_{0.5}In_{0.5}P$: Effects of strain and ordering", **S.-H. Wei** and A. Zunger, in *Proceedings of the 22nd International Conference on the Physics of Semiconductors*, edited by D. J. Lockwood, (World Scientific, Singapore, 1995), p.1268.

(83) "InAsSb/InAs: A type-I or a type-II band alignment", **S.-H. Wei** and A. Zunger, Phys. Rev. B **52**, 12039 (1995).[23]

(84) "Electronic structure theory of chalcopyrite alloys, interfaces, and ordered vacancy compounds", A. Zunger and **S.-H. Wei**, in *Proceedings of the 13th NREL PV Program Review*, edited by H. S. Ullal and C. E. Witt, (AIP, New York, 1996), p.155.

(85) "Effects of ordering on the electron effective mass and strain deformation potential in $GaInP_2$: deficiencies of the k·p model", A. Franceschetti, **S.-H. Wei** and A. Zunger, Phys. Rev. B **52**, 13992 (1995).[14]

(86) "d-band excitations in II-VI semiconductors: A broken symmetry approach to the core hole", S. B. Zhang, **S.-H. Wei** and A. Zunger, Phys. Rev. B **52**, 13975 (1995).[24]

(87) "Giant and composition dependent optical bowing coefficient in GaAsN alloy", **S.-H. Wei** and A. Zunger, **Phys. Rev. Lett. 76**, 664 (1996).[269]

(88) "Theoretical studies of chalcopyrite alloys, interfaces and ordered vacancy compounds", **S.-H. Wei** and A. Zunger, Cryst. Res. Technol. **31**, 81 (1996).[]

(89) "Fundamental optical transitions in GaN", G.D. Chen, M. Smith, J. Y. Lin, H, X, Jiang, **S.-H. Wei**, M. A. Khan and C. J. Sun, Appl. Phys. Lett. **68**, 2784 (1996).[93]

(90) "Chemical trends in band offsets of Zn and Mn-based II-VI's: d-level pinning and offset compression", **S.-H. Wei** and A. Zunger, Phys. Rev. B **53 (Rapid Communication)**, 10457 (1996).[14]

(91) "Dependence of optical properties of semiconductor alloys on long range order, strain and pressure", **S.-H. Wei**, A. Franceschetti and A. Zunger, in *Optoelectronic Materials - Ordering, Composition Modulation, and Self-Assembled Structures*, edited by E. D. Jones, A. Mascarenhas, and P. Petroff, (MRS, Pittsburgh, 1996), p.3.

(92) "Prediction of new fingerprints of ordering in $GaInP_2$ alloys", A. Franceschetti, **S.-H. Wei** and A. Zunger, in *Optoelectronic Materials - Ordering, Composition Modulation, and Self-Assembled Structures*, edited by E. D. Jones, A. Mascarenhas, and P. Petroff, (MRS, Pittsburgh, 1996), p.103.

(93) "Point-charge electrostatics in disordered alloys", C. Wolverton, A. Zunger, S. Froyen, and **S.-H. Wei**, Phys. Rev. B **54**, 7843 (1996).[18]

(94) "Valence band splittings and band offsets of AlN, GaN and InN", **S.-H. Wei** and A. Zunger, Appl. Phys. Lett. **69**, 2719 (1996).[115]

(95) "Localization and percolation in semiconductor alloys: GaAsN vs GaAsP", L. Bellaiche, **S.-H. Wei**, and A. Zunger, Phys. Rev. B **54**, 17568 (1996).[170]

(96) "Composition-dependence of interband transition intensities in semiconductor alloys: GaPN *vs* GaPAs", L. Bellaiche, **S.-H. Wei**, and A. Zunger, Phys. Rev. B **56**, 10233 (1997).[92]

(97) "Stabilization of ternary compounds via ordered array of defect pairs", S. B. Zhang, **S.-H. Wei** and Alex Zunger, **Phys. Rev. Lett. 78**, 4059 (1997).[64]

(98) "Electronic and structural anomalies in lead chalcogenides", **S.-H. Wei** and A. Zunger, Phys. Rev. B **55**, 13605 (1997).[32]

(99) "Why is $CuInSe_2$ tolerant to defects and what is the origin of ordered defect structures", A. Zunger, S. B. Zhang, and **S.-H. Wei**, in *Proceedings of the 14th NREL PV Program Review*, edited by C. E. Witt, (AIP, New York, 1997), p.63.

(100) "Point-ion vs density functional calculations of electric field gradients in ordered $GaInP_2$", **S.-H. Wei** and A. Zunger, J. Phys. Chem. **107**, 1931 (1997).[4]

(101) "Band gaps of GaPN and GaAsN alloys", L. Bellaiche, **S.-H. Wei** and A. Zunger, Appl. Phys. Lett. **70**, 3558 (1997).[92]

(102) "Bond length distribution in tetrahedral vs octahedral semiconductor alloys: The case of GaInN", L. Bellaiche, **S.-H. Wei** and A. Zunger, Phys. Rev. B **56**, 13872 (1997).[11]

(103) "Why is heavily-defected $CuInSe_2$ a good opto-electronic material: Defect physics in $CuInSe_2$", **S.-H. Wei**, S. B. Zhang, and A. Zunger, in *Proceedings of the 11th Inter. Conf. of Ternary and Multinary Compounds*, edited by R. D. Tomlinson, (AIP, New York, 1998), p. 765.[3]

(104) "Spin polarization of photoelectrons from ordered semiconductor alloys", **S.-H. Wei** in *Proceedings of the 7th Inter. Workshop on Polarized Gas Targets and Polarized Beams*, edited by R. J. Holt and M. A. Miller, (AIP, New York, 1998), p. 284.

(105) "Revisiting the defect physics in $CuInSe_2$ and $CuGaSe_2$", A. Zunger, S. B. Zhang, and **S.-H. Wei**, in *Proceedings of the 26th IEEE PV Specialist Conf.*, edited by P. A. Basore, (AIP, New York, 1998), p. 313.

(106) "The 'majority representation' of alloy electronic states", L. W. Wang, L. Bellaiche, **S.-H. Wei** and A. Zunger, **Phys. Rev. Lett. 80**, 4725 (1998).[30]

(107) "Defects physics of the $CuInSe_2$ chalcopyrite semiconductor", S. B. Zhang, **S.-H. Wei**, A. Zunger, and H. Katayama-Yoshida, Phys. Rev. B **57**, 9642 (1998).[217]

(108) "Calculated natural band offsets of all II-VI and III-V semiconductors: Chemical trends and the role of cation d orbitals", **S.-H. Wei** and A. Zunger, Appl. Phys. Lett. **72** 2011 (1998).[151]

(109) "Fingerprints of CuPt ordering in III-V semiconductor alloys: Valence band splittings, band gap reduction, and X-ray structure factors", **S.-H. Wei** and A. Zunger, Phys. Rev. B **57**, 8983 (1998).[43]

(110) "A phenomenological model for systematization and prediction of doping limits in II-VI and I-III-VI_2 compounds", S. B. Zhang, **S.-H. Wei** and A. Zunger, J. Appl. Phys. **83**, 3192 (1998).[80]

(111) "The effects of Ga addition to $CuInSe_2$ on its electronic, structural, and defect properties", **S.-H. Wei**, S. B. Zhang and A. Zunger, Appl. Phys. Lett. **72**, 3199 (1998).[62]

(112) "Trends in band gap pressure coefficients in chalcopyrite semiconductors", **S.-H. Wei**, A. Zunger, I.-H. Choi, and P. Y. Yu, Phys. Rev. B **58**, R1710 (1998). [9]

(113) "Elements of doping engineering in semiconductors", S. B. Zhang, **S.-H. Wei** and A. Zunger, in *AIP Conference Proceedings*, No. **462**, edited by M. Al-Jassim, J. P. Thornton, and J. M. Gee, (AIP, New York, 1999), p. 62.

(114) "Band structure and stability of zinc-blende-based semiconductor polytypes", **S.-H. Wei**, S. B. Zhang and A. Zunger, Phys. Rev. B **59 (Rapid Communication)**, R2478 (1999).[17]

(115) "Resonant hole localization and anomalous optical bowing in InGaN alloys", L. Bellaiche, T. Mattila, L. W. Wang, **S.-H. Wei** and A. Zunger, Appl. Phys. Lett. **74** 1842 (1999).[75]

(116) "Transmission electron microscopy investigation and first-principles calculation of the phase stability in epitaxial $CuInS_2$ and $CuGaSe_2$ films", D. S. Su and **S.-H. Wei**, Appl. Phys. Lett. **74**, 2483 (1999).[18]

(117) "Effect of Na on the electrical and structural properties of $CuInSe_2$", **S.-H. Wei**, S. B. Zhang and A. Zunger, J. Appl. Phys. **85**, 7214 (1999).[34]

(118) "Localization and anticrossing of electron levels in As-rich GaAsN alloys", T. Mattila, **S.-H. Wei** and A. Zunger, Phys. Rev. B **60 (Rapid Communication)**, R11245 (1999).[110]

(119) "Predicted band gap pressure coefficients of all diamond and zinc-blende semiconductors: The chemical trends", **S.-H. Wei** and A. Zunger, Phys. Rev. B **60**, 5404 (1999).[93]

(120) "Multi-band coupling and electronic structure of $(InAs)_n/(GaSb)_n$ superlattices", L.-W. Wang, **S.-H. Wei**, T. Mattila, A. Zunger, I. Vurgaftman, and J. R. Meyer, Phys. Rev. B **60**, 5590 (1999).[27]

(121) "Basic research opportunities in Cu-chalcopyrite photovoltaics", A. Rockett, R. N. Bhattacharya, C. Eberspacher, V. Kapur, and **S.-H. Wei**, in *Photovoltaics for the 21st Century*, edited by V. K. Kapur, R. D. McConnell, D. Carlson, G. P. Ceasar, and A. Rohatgi, (ECS, Pennington, 1999), p. 232.

(122) "Electronic structure of 'sequence mutations' in ordered $GaInP_2$ alloys", T. Mattila, **S.-H. Wei**, and A. Zunger, **Phys. Rev. Lett. 83**, 2010 (1999).[24]

(123) "Overcoming doping bottlenecks in semiconductors and wide-gap material", S. B. Zhang, **S.-H. Wei**, and A. Zunger, Physica B **274**, 976 (1999).[]

(124) "Microscopic origin of the phenomenological equilibrium 'doping limit rule' in n-type III-V semiconductors", S. B. Zhang, **S.-H. Wei**, and A. Zunger, **Phys. Rev. Lett. 84**, 1232 (2000).[37]

(125) "First-principles calculation of band-offsets, optical bowings, and defects in CdS, CdSe, CdTe and their alloys", **S.-H. Wei**, S. B. Zhang and A. Zunger, J. Appl. Phys. **87**, 1304 (2000).[48]

(126) "Band structure and stability of Ternary Semiconductor polytypes", **S.-H. Wei**, S. B. Zhang, and A. Zunger, Jpn. J. Appl. Phys. **Suppl. 39**, 237 (2000).

(127) "Long and short range ordering of $CuInSe_2$", C.-H. Chang, **S.-H. Wei**, W. Johnson, R. Bhattacharya, B. Stanbery, T. Anderson and R. Duran, Jpn. J. Appl. Phys. **Suppl. 39**, 411 (2000).

(128) "Electronic structure and stability of Spinel oxides", **S.-H. Wei**, Jpn. J. Appl. Phys. **Suppl. 39**, 251 (2000).

(129) "Structure stability and carrier localization in CdX (X=S, Se, Te) semiconductors", **S.-H. Wei** and S. B. Zhang, Phys. Rev. B **62**, 6944 (2000).[14]

(130) "ZB/WZ band offsets and carrier localization in CdTe solar cells", **S.-H. Wei**, and S. B. Zhang, in *Proceedings of 2000 NCPV Program Review Meeting*, edited by K. Ramanathan, (NTIS, Springfield, 2000), p. 293.

(131) "Local structure of $CuIn_3Se_5$", C.-H. Chang, **S.-H. Wei**, N. Leyarovska, J. W. Johnson, S. B. Zhang, B. J. Stanbery, T. J. Anderson, R. Duran, and G. Bunker in *Proceedings of 2000 NCPV Program Review Meeting*, edited by K. Ramanathan, (NTIS, Springfield, 2000), p. 247.

(132) "Observation and first-principles calculation of buried wurtzite phases in zinc-blende CdTe thin films", Y. Yan, M. M. Al-jassim, K. M. Jones, **S.-H. Wei**, and S. B. Zhang, Appl. Phys. Lett. **77**, 1461 (2000).[5]

(133) "Nitrogen solubility and nitrogen induced defect complexes in epitaxial grown GaAsN", S. B. Zhang and **S.-H. Wei**, in *Proceedings of 15th International Conference on the Physics of Semiconductors*, edited by N. Miura and T. Ando, (Osaka, 2000), p. 1493.

(134) "Intrinsic n-type vs. p-type doping asymmetry and the defect physics of ZnO", S. B. Zhang, **S.-H. Wei**, A. Zunger, Phys. Rev. B **63**, 075205 (2001).[144]

(135) "First-principles study of cation distribution in eighteen closed shell $A^{II}B_2^{III}O_4$ and $A^{IV}B^{II}O_4$ spinel oxides", **S.-H. Wei** and S. B. Zhang, Phys. Rev. B **63**, 045112 (2001).[8]

(136) "Structural and electronic properties of $ZnGeAs_2$", A. Janotti, **S.-H. Wei**, S. B. Zhang, and Sarah R. Kurtz, Phys. Rev. B **63**, 195210 (2001).[1]

(137) "Electronic structures and defect physics of Cd-based Semiconductors", **S.-H. Wei** and S. B. Zhang, in *Proceedings of 28th IEEE Photovoltaic Specialists Conference*, (IEEE, Piscataway, 2001), p. 483.

(138) "The Thermodynamics of codoping: How does it work", S. B. Zhang, **S.-H. Wei** and Yanfa Yan, Physica B **302-303**, 135 (2001).[23]

(139) "Nitrogen solubility and induced defect complexes in epitaxial GaAs:N", S. B. Zhang and **S.-H. Wei**, **Phys. Rev. Lett. 86**, 1789 (2001).[67]

(140) "Effects of ordering on physical properties of semiconductors alloys", **S.-H. Wei**, in *Spontaneous Ordering in Semiconductor Alloys*, edited by A. Mascarenhas, (Plenum, New York, 2001), p427.

(141) "Structure investigation of In-rich copper indium selenide compound semiconductor: From local structure to long range order" C.-H. Chang, **S.-H. Wei**, S. P. Ahrenkiel, J. W. Johnson, B. J. Stanbery, T. J. Anderson, S. B. Zhang, M. M. Al-Jassim, G. Bunker, E. A. Payzant, and R. Duran, in *II-VI Compound Semiconductor Photovoltaic Materials*, edited by R.W. Birkmire, R. Noufi, D. Lincot, and H.W. Schock, (MRS, Pittsburg, 2001), p. H4.3.1.

(142) "First-principles study of the stability of BN and C", A. Janotti, **S.-H. Wei**, and D. J. Singh, Phys. Rev. B **64**, 174107 (2001).[14]

(143) "Steps on As-terminated Ge(001) revisited: Theory versus experiment" S. B. Zhang, W. E. McMahon, J. M. Olson, and **S.-H. Wei**, **Phys. Rev. Lett. 87**, 166104 (2001).[7]

(144) "Reconstruction and energetics of $CuInSe_2$ surfaces", S. B. Zhang, and **S.-H. Wei**, in *Proceedings of 2001 NCPV Program Review Meeting*, edited by K. Ramanathan, (NTIS, Springfield, 2001), p. 221.

(145) "Theoretical study of doping limits of CdTe", **S.-H. Wei** and S. B. Zhang in *Proceedings of 2001 NCPV Program Review Meeting*, edited by K. Ramanathan, (NTIS, Springfield, 2001), p. 201.

(146) "Nitrogen solubility and N-induced defect complexes in epitaxial GaAs:N" S. B. Zhang and **S.-H. Wei**, Physica B **308-310**, 839 (2001).[2]

(147) "First-principles study of doping limits of CdTe", **S.-H. Wei** and S. B. Zhang, Phys. stat. sol. (b) **229**, 305 (2002).[6]

(148) "Polymophism in $CuInS_2$ epilayers: The origin of additional Raman modes", J. Alvarez-Garcia, A. Perez-Rodriguez, B. Barcones, A. Romano-Rodriguez, J. R. Morante, A. Janotti, **S.-H. Wei**, and R. Scheer, Appl. Phys. Lett. **80**, 562 (2002).[19]

(149) "Bipolar doping and band gap anomalies in delafossite transparent conductive oxides", X. Nie, S. B. Zhang, and **S.-H. Wei**, **Phys. Rev. Lett. 88**, 066405 (2002).[17]

(150) "First-principles study of transparent p-type conductive $SrCu_2O_2$ and related compounds", X. Nie, S. B. Zhang, and **S.-H. Wei**, Phys. Rev. B **65**, 075111 (2002).[5]

(151) "Self-doping of cadmium stannate in the inverse spinel structure", S. B. Zhang, and **S.-H. Wei**, Appl. Phys. Lett. **80**, 1376 (2002).[7]

(152) "Theoretical study of the effects of isovalent co-alloying of Bi and N in GaAs", A. Janotti, S. B. Zhang and **S.-H. Wei**, Phys. Rev. B **65**, 115203 (2002).[12]

(153) "Reconstruction and energetics of the polar (112) and $(\bar{1}\bar{1}\bar{2})$ versus the non-polar (220) surfaces of $CuInSe_2$", S. B. Zhang, and **S.-H. Wei**, Phys. Rev. B **65 (Rapid Communications)**, 081402 (2002).[9]

(154) "Hydrogen vibration modes in GaP:N - The pivotal role of nitrogen in stabilizing the H_2^* complex", A. Janotti, S. B. Zhang, and **S.-H. Wei**, **Phys. Rev. Lett. 88**, 125506 (2002).[17]

(155) "Origin of p-type doping difficulty in ZnO: The impurity perspective", C. H. Park, S. B. Zhang, and **S.-H. Wei**, Phys. Rev. B **66**, 073202 (2002).[27]

(156) "Chemical design of direct-gap light emitting silicon", Xuan Luo, S. B. Zhang, and **S.-H. Wei**, **Phys. Rev. Lett. 89**, 076802 (2002). [See also Research Highlights, (Nature Materials Update), August 8th, (2002).][4]

(157) "Piezoelectric coefficients of complex semiconductor alloys from first-principles: The case of $Ga_{1-x}In_xN$", A. Al-Yacoub, L. Bellaiche, and **S.-H. Wei**, **Phys. Rev. Lett. 89** 057601 (2002).[6]

(158) "The effects of hydrogen on the electronic properties of dilute GaAsN alloys", A. Janotti, S. B. Zhang, **S.-H. Wei**, and C. G. Van de Walle, **Phys. Rev. Lett. 89**, 086403 (2002).[26]

(159) "Computational design of a material for high-efficiency spin-polarized electron source", A. Janotti and **S.-H. Wei**, Appl. Phys. Lett. **81**, 3957 (2002).[3]

(160) "Electronic structure and doping of p-type transparent conducting oxides", **S.-H. Wei**, X. Nie, and S. B. Zhang, in *Proceedings of 29th IEEE Photovoltaic Specialists Conference*, (IEEE, Piscataway, 2002), p. 496.

(161) "Nitrogen-stabilized H_2^* defects in GaP:N", A. Janotti, S. B. Zhang, and **S.-H. Wei**, Mat. Res. Soc. Symp. Proc. **719**, F6.3.1 (2002).

(162) "Chemical trends of the defect formation and the doping limit in II-VI semiconductors: The case of CdTe", **S.-H. Wei** and S. B. Zhang, Phys. Rev. B **66**, 155211 (2002).[32]

(163) "Growth model for atomic ordering: The case for quadruple-period ordering in GaAsSb alloys", I. G. Batyrev, A. Norman, S. B. Zhang and **S.-H. Wei**, **Phys. Rev. Lett. 90**, 026102 (2003).[2]

(164) "Understanding ultrahigh doping: The case of boron in Silicon", X. Luo, S. B. Zhang, and **S.-H. Wei**, **Phys. Rev. Lett. 90**, 026103 (2003).[9]

(165) "Interaction between Nitrogen, hydrogen, V_{Ga} in GaAsN alloys", A. Janotti, **S.-H. Wei**, S. B. Zhang, S. R. Kurtz, and C. G. Van de Walle, Phys. Rev. B **67 (Rapid Communication)**, 161201 (2003).[17]

(166) "Electronic and magnetic properties of MnN versus MnAs", A. Janotti, **S.-H. Wei**, and L. Bellaiche, Appl. Phys. Lett. **82**, 766 (2003).[17]

(167) "Epitaxially stabilized $AgGaSe_2$ for high-efficiency spin-polarized electron source", A. Janotti, and **S.-H. Wei**, J. Phys. Chem. Solids **64**, 1881 (2003).

(168) "Breakdown of the bandgap-common-anion rule: The origin of the small band gap of InN", **S.-H. Wei**, X. Nie, I. G. Batyrev, and S. B. Zhang, Phys. Rev. B **67**, 165209 (2003).[29]

(169) "Electronic and optical properties of δ-layer $GaN/(GaAs)_n$ superlattices", X. Luo, S. B. Zhang, and **S.-H. Wei**, Phys. Rev. B **67**, 235305 (2003).[0]

(170) "Local structure of $CuIn_3Se_5$: X-ray absorption fine structure study and first-principles calculation", C.-H. Chang, **S.-H. Wei**, J. W. Johnson, S. B. Zhang, N. Leyarovska, G. Bunker, and T. J. Anderson, Phys. Rev. B. **68**, 054108 (2003).[3]

(171) "III-nitride semiconductors for photovoltaic applications", **S.-H. Wei**, in *Proceedings of 2003 NCPV and Solar Program Review Meeting*, edited by S. Asher and R. Matson, NREL/CD-520-33586, p. 712.

(172) "Design of shallow donor levels in Diamond by isovalent-donor coupling", D. Segev and **S.-H. Wei**, **Phys. Rev. Lett. 91**, 126406 (2003).[17]

(173) "Band structure and fundamental optical transitions in wurtzite AlN", J. Li, K. B. Nam, M. L. Nakami, J. Y. Lin, H. X. Jiang, P. Carrier and **S.-H. Wei**, Appl. Phys. Lett. **83**, 5163 (2003).[17]

(174) "Donor-donor Binding in Semiconductors: Engineering shallow donor levels for ZnTe", A. Janotti, **S.-H. Wei**, and S. B. Zhang, Appl. Phys. Lett. **83**, 3522 (2003).[1]

(175) "Effects of covalency, p-d coupling and epitaxial strain on the band offsets of II-VI semiconductors", D. Segev and **S.-H. Wei**, Phys. Rev. B **68**, 165336 (2003).[2]

(176) "An overview of research into transparent conducting oxides at NREL", T. J. Coutts, X. Li, D. S. Ginley, D. L. Young, J. D. Perkins, S.-H. Wei, X. Nie, and S. B. Zhang, in *Proc. 10th Int. Ceramics Congress and 3rd Forum on New Materials*, edited by P. Vincenzini, P. 1061 (2003).

(177) "Defects in GaInNAs: What we have learned so far", A. J. Ptak, S. R. Kurtz, S. W. Johnston, D. J. Friedman, J. F. Geisz, J. M. Olson, W. E. McMahon, A. E. Kibbler, C. Kramer, M. Yong, **S.-H. Wei**, S. B. Zhang, A. Janotti, P. Carrier, R. S. Crandall, B. M. Keys, P. Dippo, A. G. Norman, W. K. Metzger, R. K. Ahrenkiel, R. C. Reedy, L. Gedvilas, and B. To, in *Proceedings of 2003 NCPV and Solar Program Review Meeting*, edited by S. Asher and R. Matson, NREL/CD-520-33586, p. 202.

(178) "Theory of defects in dilute nitrides", S. B. Zhang and **S.-H. Wei**, in *Physics and Applications of Dilute Nitrides*, Chapter 8, edited by I. Buyanova and W. Chen (Taylor & Francis, New York, 2004).

(179) "Surface energy and the common dangling bond rule for semiconductors", S. B. Zhang, and **S.-H. Wei**, **Phys. Rev. Lett. 92** 086102 (2004).[5]

(180) "Isoelectronic oxygen-related defect in CdTe crystals investigated using thermoelectric effect spectroscopy", S. A. Awadalla, Alan W. Hunt, K. G. Lynn, H. Glass, C. Szeles, and **S.-H. Wei**, Phys. Rev. B. **69**, 075210 (2004).[3]

(181) "Doping by large size-mismatched impurities: The microscopic origin for p-type arsenic or antimony doped zinc-oxide", S. Limpijumnong, S. B. Zhang, **S.-H. Wei**, and C. H. Park, **Phys. Rev. Lett. 92**, 155504 (2004).[34]

(182) "Quadruple-period ordering in MBE GaAsSb alloys", I. G. Batyrev, A. G. Norman, S. B. Zhang, and **S.-H. Wei**, in *Spontaneous Ordering of Semiconductor Alloys*, edited by R. S. Goldman, R. Noetzle, A. G. Norman, and G. B. Stringfellow, (MRS, Pittsburgh, 2004), Vol. 794, T10.5.

(183) "Overcoming the doping bottleneck in semiconductors", **S.-H. Wei**, Comp. Mater. Sci. **30**, 337 (2004).[12]

(184) "Effect of Zn on the cation vacancy-oxygen pair in CdZnTe crystals", S. A. Awadalla, K. G. Lynn, **S.-H. Wei**, and C. Szeles, Phys. Rev. B **70**, 245213 (2004).

(185) "Effects of N on the electronic structures of H defects in III-V semiconductors", A. Janotti, S. B. Zhang, **S.-H. Wei**, and C. G. Van de Walle, Optical Materials **25** 261 (2004).[]

(186) "Hole-mediated stabilization of cubic GaN", G. M. Dalpian and **S.-H. Wei**, **Phys. Rev. Lett.**, **93**, 216401 (2004).[5]

(187) "Calculated spin-orbit splitting of all diamond and zinc-blende semiconductors: Effects of $p_{1/2}$ orbitals and chemical trends", P. Carrier and **S.-H. Wei**, Phys. Rev. B **70** 035212 (2004).[6]

(188) "Effect of alloying, ordering and strain on the exchange parameters of II-VI dilute magnetic semiconductors", D. Segev and **S.-H. Wei**, Phys. Rev. B **70**, 184401 (2004).[1]

(189) "Theory of Mn supersaturation in Si and Ge", Xuan Luo, S. B. Zhang, and **S.-H. Wei**, Phys. Rev. B **70**, 033308 (2004).[4]

(190) "Energetics and electronic structure of stacking faults in ZnO", Y. Yan, G. M. Dalpian, M. M. Al-jassim, and **S.-H. Wei**, Phys. Rev. B. **70**, 193206 (2004).[1]

(191) "Physics of defects and hydrogen in dilute nitrides", S. B. Zhang, A. Janotti, **S.-H. Wei**, and C. G. Van de Walle, IEE Proc.-Optoelectro. **151**, 369 (2004).[1]

(192) "Theoretical study of the band gap anomaly of InN", P. Carrier and **S.-H. Wei**, J. Appl. Phys. **97**, 033707 (2005).[19]

(193) "Stabilization of zinc-blende semiconductors through 3d impurities and holes", G. M. Dalpian and **S.-H. Wei**, in *Proceedings of 27th International Conference of Physics of Semiconductors*, edited by J. Menendez and C. G. Van de Walle, (AIP, New York, 2005), p. 225.

(194) "Band structure parameters of the nitrides: The origin of the small band gap of InN", P. Carrier and **S.-H. Wei**, in *Proceedings of 27th International Conference of Physics of Semiconductors*, edited by J. Menendez and C. G. Van de Walle, (AIP, New York, 2005), p. 287.

(195) "Vibrational and crystalline Properties of polymorphic $CuInC_2$ (C=Se,S) chalcogenides", J. Alvarez-Garcia, B. Barcones, A. Perez-Rodriguez, A. Romano-Rodriguez, J. R. Morante, A. Janotti, **S.-H. Wei** and R. Scheer, Phys. Rev. B **71**, 054303 (2005).[2]

(196) "First-principles study of Mn-induced local magnetic moments in host semiconductors", Shi-Hao Wei, X. G. Gong, G. M. Dalpian, and **S.-H. Wei**, Phys. Rev. B **71**, 144409 (2005).[4]

(197) "Hydrogen Passivation effect in nitrogen-doped ZnO thin film", X. Li, B. Keyes, S. Asher, S. B. Zhang, **S.-H. Wei**, and T. J. Coutts, S. Limpijumnong, C. G. Van de Walle, Appl. Phys. Lett. **86**, 122107 (2005).[11]

(198) "Structure-derived electronic and optical properties of transparent conducting oxides", D. Segev and **S.-H. Wei**, Phys. Rev. B **71**, 125129 (2005).[1]

(199) "Impurity-Stabilized Zinc-blende phase of wurtzite compounds", G. M. Dalpian and **S.-H. Wei**, J. Phys. Chem. Solids **66**, 2008 (2005).[0]

(200) "Electronic and optical properties of spinel TCOs: $SnZn_2O_4$, $SnCd_2O_4$, and $CuIn_2O_4$", **S.-H. Wei** and D. Segev, in *Proceedings of DOE Solar Energy Technologies Program Review Meeting 2004*, p. 32.

(201) "Transition from ferromagnetism to antiferromagnetism in $Ga_{1-x}Mn_xN$", G. M. Dalpian and **S.-H. Wei**, J. Appl. Phys. **98**, 083905 (2005).[1]

(202) "Defect Properties of $CuInSe_2$ and $CuGaSe_2$", **S.-H. Wei** and S. B. Zhang, J. Phys. Chem. Solids **66**, 1994 (2005).[1]

(203) "Evolution of structural properties and formation of N-N split interstitials in $GaAs_{1-x}N_x$ alloys", P. Carrier, **S.-H. Wei**, S. B. Zhang, and S. Kurtz, Phys. Rev. B **71**, 165212 (2005).[5]

(204) "Photoinduced cation interstitial diffusion in II-VI semiconductors", G. M. Dalpian and **S.-H. Wei**, Phys. Rev. B **72**, 075208 (2005).[2]

(205) "Substitutional diatomic molecule NO, NC, CO, N_2 and O_2, their vibrational frequencies, and the effects on p-doping of ZnO", S. Limpijumnong, X. Li, **S.-H. Wei**, and S. B. Zhang, Appl. Phys. Lett. **86**, 211910 (2005).[0]

(206) "Stability of DX center in GaAs quantum dots", J. Li, **S.-H. Wei**, L.-W. Wang, **Phys. Rev. Lett. 94**, 185501 (2005).[4]

(207) "Step structures on MOVCD grown III-V phosphide (001) surfaces: How do steps and Sb affect CuPt ordering of GaInP", I. G. Batyrev, W. E. McMahon, S. B. Zhang, J. M. Olson, and **S.-H. Wei**, **Phys. Rev. Lett. 94**, 096101 (2005).[0]

(208) "Electron-induced stabilization of ferromagnetism in GaGdN", G. M. Dalpian, and **S.-H. Wei**, Phys. Rev. B **72**, 115201 (2005).[3]

(209) "Oxygen vacancy mediated adsorption and reactions of molecular oxygen on the ZnO(10-10) surface", Y. Yan, M. M. Al-Jassim, and **S.-H. Wei**, Phys. Rev. B **(Rapid Communication) 72**, 161307 (2005).[1]

(210) "Dielectric function and electronic band structure of lead zirconate titanate", H. Lee, Y. S. Kang, S.-J. Cho, B. Xiao, H. Morkoc, T. D. Kang, J. Li, **S.-H. Wei**, P. Snyder, J. T. Evans, J. Appl. Phys. **98**, 094108 (2005).[0]

(211) "Mutual passivation of donors and isovalent impurities in dilute GaAsN Alloys", J. Li, P. Carrier, **S.-H. Wei**, S.-S. Li, and J.-B. Xia, **Phys. Rev. Lett. 96**, 035505 (2006).[0]

(212) "Electronic structure of semiconductor nanocrystals", J. Li, L.-W. Wang, and **S.-H. Wei**, Chinese J. Semiconductors **27**, 191 (2006).[0]

(213) "Novel approach to tune the physical properties of organic-inorganic hybrid semiconductors", Y. Zhang, G. M. Dalpian, B. Fluegel, **S.-H. Wei**, A. Mascarenhas, X.-Y. Huang, J. Li, and L. W. Wang, **Phys. Rev. Lett. 96**, 026405 (2006).[1]

(214) "Alignment of isovalent impurity levels: Oxygen impurity in II-VI semiconductors", J. Li and **S.-H. Wei**, Phys. Rev. B **(Rapid Communications) 73**, 041201R (2006).[0]

(215) "Impurity effect in ZnO and nitrogen doped ZnO thin films fabricated by MOCVD", X. Li, S. Asher, S. Limpijumnong, B. Keyes, C. L. Perkins, H. Moutinho, J. Luther, S. B. Zhang, **S.-H. Wei**, and T. J. Coutts, J. Crystal Growth **287** 94 (2006).[0]

(216) "Phenomenological band structure model of magnetic coupling in semiconductors", G. M. Dalpian, **S.-H. Wei**, X. G. Gong, A. J. R. da Silva and A. Fazzio, Solid State Commun. **138**, 353 (2006).[4]

(217) "*Ab-initio* calculation of hydrostatic absolute deformation potential of semiconductors", Y.-H. Li, X. G. Gong, and **S.-H. Wei**, Appl. Phys. Lett. **88**, 042104 (2006).[1]

(218) "Synthesis and characterization of nitrogen-doped ZnO films grown by MOCVD", T. J. Coutts, X. Li, T. M. Barnes, B. M. Keyes, C. L. Perkins, S. E. Asher, S. B. Zhang, **S.-H. Wei**, and S. Limpijumnong, **Chapter 3**, in *Zinc Oxide Bulk, Thin-Films, and Nanostructures*, edited by C. Jagadish and S. J. Pearton, (Elsevier Science, New York, 2006), p. 43.

(219) "Probing deactivation in nitrogen doped ZnO by vibrational signatures: A first-principles study", S. Limpijumnong, X. Li, **S.-H. Wei**, and S. B. Zhang, Physica B **376-377**, 686 (2006).[0]

(220) "Electron-mediated ferromagnetism and negative $s-d$ exchange splitting in semiconductors", G. M. Dalpian and **S.-H. Wei**, Phys. Rev. B **73**, 245204 (2006).[0]

(221) "Bistability of cation interstitials in II-VI semiconductors", **S.-H. Wei** and G. M. Dalpian, in *Proceedings of DOE Solar Energy Technologies Program Review Meeting 2005.*

(222) "Band gap of Hg chalcogenides: Symmetry-reduction-induced band gap opening of materials with inverted band structures", C.-Y. Moon and **S.-H. Wei**, Phys. Rev. B **74**, 045205 (2006).

(223) "Impurity-induced phase stabilization of semiconductors", G. M. Dalpian, Y. Yan, and **S.-H. Wei**, Appl. Phys. Lett. **89**, 011907 (2006).

(224) "Study of phase selectivity of organic-inorganic hybrid semiconductors", C.-Y. Moon, G. M. Dalpian, Y. Zhang, **S.-H. Wei**, X.-Y. Huang, and J. Li, Chem. Mater. **18**, 2805 (2006).

(225) "Carrier-mediated stabilization of ferromagnetism in semiconductors: holes and electrons", G. M. Dalpian and **S.-H. Wei**, phys. stat. sol. (b) **243** 2170 (2006).

(226) "First-principles study of native defects in anatase TiO_2", S. Na-Phattalung, M. F. Smith, K. Kim, M.-H. Du, **S.-H. Wei**, S. B. Zhang, and S. Limpijumnong, Phys. Rev. B **73**, 125205 (2006).

(227) "*Ab initio* all-electron calculation of absolute volume deformation potentials of IV-IV, III-V, and II-VI semiconductors: The chemical trends", Y.-H. Li, X. G. Gong, and **S.-H. Wei**, Phys. Rev. B **73**, 245206 (2006).

(228) "Design of shallow acceptors in ZnO: First-principles band-structure calculations", J. Li, **S.-H. Wei**, S.-S. Li, Jian-Bai Xia, Phys. Rev. B **74** **(Rapid Communication)**, 081201(R) (2006).

(229) "Unintentional doping and compensation effects of carbon in metal-organic chemical-vapor deposition fabricated ZnO thin films" X. Li, S. E. Asher, S. Limpijumnong, S. B. Zhang, **S.-H. Wei**, T. M. Barnes, T. J. Coutts, and R. Noufi, J. Vac. Sci. Technol. A **24**, 1213 (2006).

(230) "Ordering induced direct/indirect transitions in semiconductor alloys", C.-Y. Moon, J. Li, **S.-H. Wei**, A. T.-L. Lim and Y. P. Feng, Phys. Rev. B **74**, 205203 (2006).

(231) "Doping of ZnO by group-Ib elements", Y. Yan, M. M. Al-Jassim, and **S.-H. Wei**, Appl. Phys. Lett. **89** 181912 (2006).

(232) "Band gap bowing coefficients in large size-mismatched II-VI alloys: first-principles calculations", C.-H. Moon, **S.-H. Wei**, Y. Z. Zhu, and G. D. Chen, Phys. Rev. B **74**, 233202 (2006).

(233) "Study of defect levels in CdTe using thermoelectric effect spectroscopy", R. Soundararajan, K. G. Lynn, S. Awadallah, C. Szeles, and **S.-H. Wei**, J. Electronic Mater. **35**, 1333 (2006).

(234) "Superhard pseudocubic BC_2N superlattices", S. Chen, X. G. Gong, and **S.-H. Wei**, **Phys. Rev. Lett. 98**, 015502 (2007).

(235) "Possible approach to overcome the doping polarity in wide-band-gap semiconductors", Y. Yan, J. Li, **S.-H. Wei**, and M. M. Al-Jassim, **Phys. Rev. Lett. 98**, 135506 (2007).

(236) "Phase control of Cu_xTe film and its effects on CdS/CdTe solar cell", X. Wu, J. Zhou, A. Duda, Y. Yan, G. Teeter, S. Asher, W. K. Metzger, S. Demtsu, **S.-H. Wei**, and R. Noufi, Thin Solid Films **515**, 5798 (2007).

(237) "Chemical Trends of defect formation in Si quantum dots: The case of group-III and group-V dopants", Q. Xu, J.-W. Luo, S.-S. Li, J.-B. Xia, J. Li and **S.-H. Wei**, Phys. Rev. B **75**, 235304 (2007).

(238) "Band structure anomaly of chalcopyrite semiconductors $CuGaX_2$ versus $AgGaX_2$ (X=S and Se) and their alloys", Shiyou Chen, X. G. Gong and **S.-H. Wei**, Phys. Rev. B **75**, 205209 (2007).

(239) "Stability and electronic structures of Cu_xTe", J. L. F. Da Silva, **S.-H. Wei**, J. Zhou, and X. Wu, Appl. Phys. Lett. **91**, 091902 (2007).

(240) "Atomic structure of In_2O_3-ZnO systems", Y. Yan, J. L. F. Da Silva, **S.-H. Wei**, and M. M. Al-Jassim, Appl. Phys. Lett. **90**, 261904 (2007).

(241) "Effects of the wavefunction localization in $Al_xIn_yGa_{1-x-y}N$ quaternary alloys", F. Wang, S.-S. Li, J.-B. Xia, H. X. Jiang, J. Y. Lin, J. Li, and **S.-H. Wei**, Appl. Phys. Lett. **91**, 061125 (2007).

(242) "The mechanism of J-V 'roll-over' in CdS/CdTe Devices", J. Zhou, X. Wu, Y. Yan, S. Asher, J. DL. F. Da Silva, **S.-H. Wei**, L. Weinhardt, M. Bar, and C. Heske, Mater. Res. Soc. Symp. Proc. **1012**, Y13-03 (2007).

(243) "An electronic structure study of the Co-Fe-Al oxide spinel system", A. Walsh, **S.-H. Wei**, Y. Yan, M. M. Al-Jassim, J. A. Turner, M. Woodhouse, and B. A. Parkinson, Phys. Rev. B **76**, 165119 (2007).

(244) "Doping Asymmetry in wide-band gap semiconductors: Origins and Solutions", Y. Yan and **S.-H. Wei**, Phys. Stat. Sol. (b) (Review Article) (in press).

(245) "Filling the green gap: A first-principles study of the LiMgZnN alloy system", A. Walsh and **S.-H. Wei**, Phys. Stat. Sol. (b) (in press).

(246) "Electrical benign behavior of grain-boundary in polycrystalline $CuInSe_2$", Y. Yan, C.-S. Jiang, R. Noufi, **S.-H. Wei**, H. R. Moutinho, and M. M. Al-Jassim, Phys. Rev. Lett. **99**, 235504 (2007).

(247) "Density-functional theory study of the effects of atomic doping on the band edges of monoclinic WO_3", M. H. Huda, Y. Yan, C.-Y. Moon, **S.-H. Wei**, and M. M. Al-Jassim, submitted to Phys. Rev. B.

(248) "The asymmetry of adsorption of oxygen at wurtzite AlN (0001) and (000-1) surfaces" H. Ye, G. Chen, Y. Zhu, and **S.-H. Wei**, Phys. Rev. B **77**, 033302 (2008).

(249) "Large-scale ab initio study of size, shape, and doping effects on electronic structure of nanocrystals", J. Li and **S.-H. Wei**, Book Chapter (in press).

(250) "Reply to the Comment on 'Superhard pseudocubic BC_2N superlattices"', S. Chen, X. G. Gong and **S.-H. Wei**, Phys. Rev. Lett. **99**, 159602 (2007).

(251) "Theoretical study of stability and electronic structure of Li(Mg,Zn)N alloys: A candidate for solid state lighting", A. Walsh and **S.-H. Wei**, Phys. Rev. B. **76**, 195208 (2007).

(252) "Origin of doping bottleneck in semiconductor quantum dots", J. Li, **S.-H. Wei**, S.-S. Li, and J.-B. Xia, Submitted to Phys. Rev. B.

(253) "Theoretical study of crystal structures and hardness of BC_2N and BC_4N alloys", S. Chen, X. G. Gong and **S.-H. Wei**, Phys. Rev. B (in press).

(254) "The nature of the band gap in In_2O_3 revealed by first-principles calculations and X-ray spectroscopy", A. Walsh, J. F. Da Silva, **S.-H. Wei**, C. Korber, A. Klein, L. F. J. Piper, A. DeMasi, K. E. Smith, G. Panaccione, P. Torelli, D. J. Payne, A. Bourlange, and R. G. Egdell, Submitted to Phys. Rev. Lett.

(255) "Ground state structure of coherent lattice-mismatched zinc-blende $A_{1-x}B_xC$ (x=0.25, 0.75) semiconductor alloys", S. Chen, X. G. Gong, and **S.-H. Wei**, Submitted to Phys. Rev. B.

(256) "Mg acceptor energy level in AlGaInN quaternary alloys: An approach to overcome the p-type doping bottleneck in nitrides", F. Wang, J. Li, S.-S. Li, J.-B. Xia, and **S.-H. Wei**, Submitted to Appl. Phys. Lett.

(257) "Rules of the structure formation of the homologous $InMO_3(ZnO)_n$ compounds", J. L. F. Da Silva, Y. Yan, and **S.-H. Wei**, Submitted to Phys. Rev. Lett.

(258) "Origin of the structural and magnetic anomaly of the layered compound $SrFeO_2$: A Density Functional Investigation ", H. J. Xiang, **S.-H. Wei**, and M.-H. Whangbo, Submitted to Phys. Rev. Lett.

(259) "Determination of phase ratio in polymorphic materials by X-ray absorption spectroscopy: The case of anatase and rutile phase mixture in TiO_2", M. F. Smith, W. Klysubun, S. Kityakarn and A. Worayingyong, S. B. Zhang, **S.-H. Wei**, D. Onkaw, P. Sonngsiriritthigul, S. Rujirawat, and S. Limpijumnong, Submitted to Appl. Phys. Lett.

(260) "Electronic, energetic and chemical effects of intrinsic defects and Fe-doping of $CoAl_2O_4$: A DFT+U study ", A. Walsh, Y. Yan, M. M. Al-Jassim, and **S.-H. Wei**, Submitted to J. Phys. Chem. C.

(258) "Band coupling model of electron and hole mediated ferromagnetism in semiconductors: The case of GaN ", **S.-H. Wei** and G. M. Dalpian, Submitted to SPIE.