

PUBLICATION LIST of Keivan Esfarjani

Book:

- “Computational Materials Science; from Ab initio to Monte Carlo Methods”, K. Ohno, K. Esfarjani and Y. Kawazoe; Solid State Series, vol. **129**, Springer-Verlag, Berlin, Germany (1999).

Review Articles:

1. “An all-electron first-principles molecular dynamics method and a possibility of its application to atomistically disordered systems”, K. Ohno, Y. Maruyama, H. Kamiyama, E. Bei, K. Shiga, Z.-Q. Li, K. Esfarjani, and Y. Kawazoe; **Review article** *Advanced Materials Research* **1**, p. 210-219 (1998).
2. “Electronic, transport and mechanical properties of carbon nanotubes” K. Esfarjani, Amir A. Farajian, Yuichi Hashi, and Yoshiyuki Kawazoe; **Review article** *Clusters and Nanomaterials, Springer-Verlag, Berlin, Germany* p.187-220 (2001).
3. “Computer simulations on clusters: Structures and electronic properties” V. Kumar, K. Esfarjani, and Y. Kawazoe; **Review article** *Clusters and Nanomaterials, Springer-Verlag, Berlin, Germany* p.9-88 (2001).
4. “The nanostructure of C₆₀ photopolymers” J. Onoe, T. Nakayama, A. Nakao, Y. Hashi, K. Esfarjani, K. Ohno, Y. Kawazoe, M. Aono, and K. Takeuchi; **Review article** *Clusters and Nanomaterials, Springer-Verlag, Berlin, Germany* p.135-169 (2001).
5. “Statistical Mechanical Modeling and its Application to Nanosystems” K. Esfarjani and G. A. Mansoori; **Review article** to appear in the *Handbook of Theoretical and computational Nanotechnology*; Vol X, Chap. 16, p. 1-45 (2005).

Journal Articles and Conference Proceedings:

1. “Path integrals, Disorder and Quantum Hall Oscillations” K. Esfarjani, H. R. Glyde and V. Sayakanit; *Proceedings of the 3rd International Conference on Path Integrals from mev to Mev*, 176-194 (1989).
2. “Disorder, Screening and Quantum Hall Oscillations” K. Esfarjani, H. R. Glyde and V. Sayakanit; *Phys. Rev. B.* **41**, 1042 (1990).
3. “Solidification of the two-dimensional electron gas in high magnetic fields” K. Esfarjani and S. T. Chui; *Phys. Rev. B.* **42**, 10758 (1990).
4. “Finite temperature transport of a pinned two-dimensional electron system” S. T. Chui and K. Esfarjani; *Phys. Rev. Lett.* **66**, 652 (1991).

5. "A mechanism for quantum melting in two dimensions"
S. T. Chui and K. Esfarjani; *Europhys. Lett.* **14**, 361 (1991).
6. "Self-consistent phonon and magnetophonon and cubic anharmonic corrections of the 2D electron lattice"
K. Esfarjani and S. T. Chui; *J. Phys. Condens. Matter* **3**, 5825 (1991).
7. "Finite-temperature two-dimensional Wigner transition"
S. T. Chui and K. Esfarjani; *Phys. Rev. B* **44**, 11498 (1991).
8. "Shear modulus of the magnetophonon wavefunction"
K. Esfarjani and S. T. Chui; *Solid State Com.* **79**, 387 (1991).
9. "Dislocation waves in a 2-dimensional Coulomb lattice"
K. Esfarjani, S. T. Chui and Qiu Xiu; *Phys. Rev. B* **46**, 4638 (1992).
10. "Electronic Properties of $C_{58}NB$ Fullerene Solids"
K. Esfarjani, B. L. Gu, Y. Maruyama, K. Ohno, and Y. Kawazoe; *Materials Research Society Symposium Proceedings*, 225 (Spring 1994).
11. "Search for the ground state of $C_{60}B_{10}$ "
K. Esfarjani, K. Ohno, and Y. Kawazoe; *Materials Research Society Symposium Proceedings*, 229 (Fall 1994).
12. "Band Structure and Chemical Bonding in $C_{58}NB$ Fullerenes"
K. Esfarjani, K. Ohno, and Y. Kawazoe; *Phys. Rev. B.* **50**, 17830 (1994).
13. "A bilayer of Wigner crystal in the harmonic approximation"
K. Esfarjani and Y. Kawazoe; *Jour. Phys. Condens. Mat.* **7**, 7217 (1995).
14. "Site occupation reversal in Fe-Cr σ phase"
M. Sluiter, K. Esfarjani, and Y. Kawazoe; *Phys. Rev. Lett.* **75**, 3142 (1995).
15. "Effect of orientation on the band structure of $C_{58}NB$ hetero-fullerenes in fcc solid phase",
K. Esfarjani, K. Ohno, and Y. Kawazoe; *Solid State Com.* **97**, 539 (1996).
16. "Phase Stability of the Sigma Phase in Fe-Cr Based Alloys"
M. Sluiter, K. Esfarjani, and Y. Kawazoe; *Materials Research Society Symposium Proceedings*, **408**, 369 (1996).
17. "Electronic structure of $C_{58}BN$ clusters"
K. Esfarjani, K. Ohno, and Y. Kawazoe; *Proceedings of the ISSPIC conference in Kobe*, Surface Rev. Lett. **3**,747 (1996).
18. "Electronic structure of C_{240} rings"
Y. Hashi, K. Esfarjani, S. Itoh, S. Ihara, and Y. Kawazoe; *MRS-J Symposium I Proceedings, Trans. Mat. Res. Soc. Japan*, **20**, 486 (1996).
19. "Ab-initio molecular dynamics simulations for collision between C_{60}^- and alkali-metal ions: A possibility of LiC_{60} "
K. Ohno, Y. Maruyama, K. Esfarjani, Y. Kawazoe and M. Niwano; *Phys. Rev. Lett.* **76**, 3590 (1996).

20. "Tight-binding molecular dynamics simulation of fullerene collision processes,"
Y. Hashi, K. Esfarjani, K. Ohno and Y. Kawazoe; *Sci. Rep. RITU*, **3**, A41,
p.171-173, (1996).
21. "Ab-initio Molecular Dynamics Simulation of Li Insertion in C_{60} "
Y. Maruyama, K. Ohno, K. Esfarjani, and Y. Kawazoe; *Sci. Rep. RITU*, **3**, A41,
p.183-186, (1996).
22. "Stability and vibrational spectra of C_{240} isomers"
K. Esfarjani, Y. Hashi, S. Itoh, S. Ihara, and Y. Kawazoe; *Z. für Phys. D*, **41**,
73, (1997).
23. "Surface Reconstruction of Si (001) by Genetic Algorithms and Simulated An-
nealing Methods"
R. T. Fu, K. Esfarjani, Y. Hashi, J. Wu and Y. Kawazoe; *Sci. Rep. RITU*, p.
77-81, January (1997).
24. "Application of computational physics to the design of new nanoscale devices:
nanodiodes and nano-transistors"
K. Esfarjani, *Invited talk at the IPMM'97 Conference Proceedings*, Vol. 1, p.
171-176 (1997).
25. "Simulated Annealing of Small Silicon Clusters by Tight-Binding"
K. Esfarjani, Y. Hashi and Y. Kawazoe; *Nuclus97 Conference Proceedings, Sim-
ilarities and differences between atomic nuclei and clusters*, p. 403-406 (AIP no.
416, 1997).
26. "Tight-binding method for Cu clusters; ground state studies of $Cu_3 - Cu_{12}$ "
A. Taneda, K. Esfarjani, Y. Hashi and Y. Kawazoe; *Nuclus97 Conference Proceed-
ings, Similarities and differences between atomic nuclei and clusters*, p. 471-474
(AIP no. 416, 1997).
27. "Efficiency of Parallel Machine for Large-Scale Simulation in Computational Physics"
H. Mizuseki, K. Esfarjani, Z.Q. Li, K. Ohno, Y. Akiyama, Y. Ichinoseki, and Y.
Kawazoe. *High Performance Computing (Lecture Notes Comput. Sci., 1336)*,
381, (1997).
28. "Vibrational modes and IR analysis of neutral photopolymerized C_{60} dimers"
K. Esfarjani, Y. Hashi, J. Onoe, K. Takeuchi, and Y. Kawazoe; *Phys. Rev. B*,
57 , 223 (1998).
29. "Transport properties of doped carbon nanotubes"
A. A. Farajian, K. Esfarjani, Y. Hashi and Y. Kawazoe; *Proceedings of the special
symposium on advanced materials, Nagoya, Japan, in Advanced Materials* **4** p.15-
18 (1998).
30. "Nanotube diodes"
K. Esfarjani, A.A. Farajian, Y. Hashi and Y. Kawazoe; *Proceedings of the 2nd
Cluster Symposium*, p. 145-148, April 1998, Osaka, Japan.
31. "Tight-binding parametrization of transition metal elements from LCAO ab-initio
Hamiltonians"
A. Taneda, K. Esfarjani, Z. Q. Li and Y. Kawazoe; *Computational Materials
Science*, **9**, 343 (1998).

32. "Self-consistent tight-binding formalism for charged systems"
K. Esfarjani and Y. Kawazoe; *Jour. Phys. Condens. Mat.*, **10**, 8257 (1998).
33. "In situ FTIR, XPS, and STM studies of the nano-structure of a photopolymerized C₆₀ film"
J. Onoe, T. Nakayama, A. Nakao, Y. Hashi, K. Esfarjani, Y. Kawazoe, M. Aono, and K. Takeuchi, *ISIC-10 Proceedings, Mol. Cryst. Liq. Cryst.* **340**, 689 (1999).
34. "Genetic Algorithms"
K. Esfarjani, K. Shida, K. Ohno and Y. Kawazoe; *Materia Japan*, **37**, no. 10, p. 893, (1998). (in Japanese)
35. "Electronic and transport properties of N-P doped nanotubes"
K. Esfarjani, A. A. Farajian, Y. Hashi, and Y. Kawazoe; *Appl. Phys. Lett.* **74**, 79 (1999).
36. "The three-fermion problem in two and three dimensions; a unified variational approach"
A. A. Farajian, K. Esfarjani and Y. Kawazoe; *J. Phys. B* **32**, 749 (1999).
37. "FT-IR and FT-MS studies of a photoirradiated K_xC₆₀ film"
J. Onoe, Y. Hashi, K. Esfarjani, Y. Kawazoe, and K. Takeuchi, *Eur. Phys. J. D*, **9**, 363 (1999).
38. "Ground state structure of silicon clusters by SA and GA methods"
K. Esfarjani Y. Hashi, K.Shida and Y. Kawazoe; *Proceedings of CIMTEC'98, Computational Modeling and Simulation of Materials, Techna*, (1999).
39. "Electronic properties of doped nanotubes"
K. Esfarjani, A. A. Farajian, Y. Hashi and Y. Kawazoe; *Proceedings of CIMTEC'98, Computational Modeling and Simulation of Materials, Techna*, (1999).
40. "The renormalized-interaction method: a new order-N algorithm"
K. Esfarjani, and Y. Kawazoe; *Proceedings of the 3rd Cluster Symposium, Tokyo Met. Univ.*, p. 169-171, (May 12-14, 1999).
41. "Optimized geometries and charge transfer in Ga and As dimers on Si surface: an ab initio study"
A.A. Farajian, K. Esfarjani, and Y. Kawazoe; *Proceedings of the 3rd Cluster Symposium, Tokyo Met. Univ.*, p. 115-117, (May 12-14, 1999).
42. "Localized-basis-set optimization"
K. Esfarjani, Amir A. Farajian and Y. Kawazoe; *Comp. Mat. Sci.* **15**, 351 (1999).
43. "Ab initio study of dopant insertion into carbon nanotubes"
A. A. Farajian, K. Ohno, K. Esfarjani, Y. Maruyama, and Y. Kawazoe; *J. Chem. Phys.* **111**, 2164 (1999).
44. "Nonlinear coherent transport through doped nanotube junctions"
A. A. Farajian, K. Esfarjani, and Y. Kawazoe; *Phys. Rev. Lett.* **82**, 5084 (1999).
45. "In-situ Infrared Spectroscopy of a Photoirradiated Potassium-doped C₆₀ film"
J. Onoe, Y. Hashi, K. Esfarjani, T. Hara, Y. Kawazoe, and K. Takeuchi; *Chem. Phys. Lett.* **315**, 19 (1999).

46. "AC response of doped nanotube junctions"
K. Esfarjani, A. A. Farajian, S. T. Chui, and Y. Kawazoe; *Proceedings of the third Sanken International Symposium, Osaka, Japan*, p. 164 (March 2000).
47. "Elastic interaction between self-assembled quantum dots"
S. Vannarat, K. Esfarjani, and Y. Kawazoe; *Proceedings of the third Sanken International Symposium, Osaka, Japan*, p. 138 (March 2000).
48. "Electronic Structure of Single and Double Layer Graphene Tubules by the Folding Method"
A. Tajik, K. Esfarjani, and F. Ebrahimi; *Proceedings of the Condensed Matter workshop, IASBS, Zanjan, Iran* (April 2000).
49. "Electronic properties of carbon onions"
K. Esfarjani, Y. Hashi, and Y. Kawazoe; *Proceedings of the Condensed Matter workshop, IASBS, Zanjan, Iran* (April 2000).
50. "Effect of inter-island interaction on the growth of self-assembled quantum dots"
S. Vannarat, S. T. Chui, K. Esfarjani, and Y. Kawazoe; *Proceedings of the 25th International Conference on the Physics of Semiconductors, Osaka, Japan* (Sept. 2000).
51. "In situ FTIR, XPS and STM studies of the nano-structure of a photopolymerized C₆₀ film",
J. Onoe, T. Nakayama, A. Nakao, Y. Hashi Y, K. Esfarjani, Y. Kawazoe, M. Aono and K. Takeuchi; *Molec. Crys. Liq. Crys.* **340** 689 (2000).
52. "Realization of an effective ultrahigh magnetic field on a nanoscale"
S. T. Chui, J. T. Wang, L. Zhou, K. Esfarjani, and Y. Kawazoe; *J. Phys. Condens. Matt.* **13**, L49 (2001).
53. "Transport properties of a nanotube-based transistor"
K. Esfarjani, A. A. Farajian, F. Ebrahimi, and Y. Kawazoe; *Euro. Phys. Jour. D* **16**(1-3) 353-355 (Sept. 2001).
54. "Phase separation in fermion droplets"
K. Esfarjani, S. T. Chui, V. Kumar, and Y. Kawazoe; *Transactions of the Materials Research Society of Japan (MRS-J)*, **26**, 1101-1104 (2001).
55. "Rotational Symmetry Selection Rule and Doping in Nanotube Transistors"
K. Esfarjani, Amir A. Farajian, Farshad Ebrahimi and Yoshiyuki Kawazoe; *Transactions of the Materials Research Society of Japan (MRS-J)*, (2001).
56. "Analysis of C60 Insertion into Single Wall Carbon Nanotube by Molecular Dynamics Simulation"
Takafumi Ishii, K. Esfarjani, Yuichi Hashi, Yoshiyuki Kawazoe and Sumio Iijima; *Proceedings of the Materials Research Society of Japan (MRS-J)*, (2001).
57. "Charge oscillation at doped nanotube junctions"
A. A. Farajian, K. Esfarjani and Y. Kawazoe; *Proceedings of the ISNM2001 International Conference*, (2001).
58. "Spin valve effect in magnetically doped nanotube-based transistors"
K. Esfarjani, Z. Chen, A. A. Farajian and Y. Kawazoe; *Proceedings of the ISNM2001 International Conference*, (2001).

59. "Analysis of C60 Insertion into Single Wall Carbon Nanotube by Molecular Dynamics Simulation"
Takafumi Ishii, K. Esfarjani, Yuichi Hashi, Yoshiyuki Kawazoe and Sumio Iijima; *Proceedings of the ISNM2001 International Conference*, (2001).
60. "Effect of Elastic interaction on self-assembled island spatial arrangement"
S. Vannarat, K. Esfarjani, S. T. Chui, and Y. Kawazoe; *Mater. Trans.* **42**(11) 2279-2282, Spec. Issue (Nov. 2001).
61. "Why the all-electron full-potential approach is suitable for calculations on fullerenes and nanotubes"
Y. Kawazoe, K. Ohno, K. Esfarjani, Y. Maruyama Y, K. Shiga, A. A. Farajian; *J. MOL. GRAPH. MODEL.* **19**(2) 270-273 (2001).
62. "Transport through Dimerized Ga and As Atomic Wires Deposited on Si(100) Substrate"
A. A. Farajian, K. Esfarjani, H. Mizuseki and Y. Kawazoe; *Proc. Intl. Symp. on Cluster Assembled Mater., IPAP Conf. Series***3**, 172-174 (2001).
63. "Calculation of diamond vacancy Hamiltonian parameters"
M. Sayyari, M. Heydari Saani, K. Esfarjani, M. A. Vesaghi; *Proceedings of the Condensed Matter workshop, IASBS, Zanjan, Iran* (April 2002).
64. "Calculation of the transmission coefficient for linear and cyclic molecules"
M. Mardaani and K. Esfarjani; *Proceedings of Sixth Condensed Matter conference of the Iranian Physical Society* (2002).
65. "Effect of disorder on the density of states using CPA"
H. Cheraghchi and K. Esfarjani; *Proceedings of Sixth Condensed Matter conference of the Iranian Physical Society* (2002).
66. "Simulation of carbon nanotube growth"
Z. Nasrollahi, N. Gorjizadeh and K. Esfarjani; *Proceedings of Sixth Condensed Matter conference of the Iranian Physical Society* (2002).
67. "Spin dynamics and magnons in a quantum dot"
M. R. Mozaffari and K. Esfarjani; *Proceedings of Sixth Condensed Matter conference of the Iranian Physical Society* (2002).
68. "Screening, charge and magnetization profiles in junctions"
A. A. Shokri and K. Esfarjani; *Proceedings of Sixth Condensed Matter conference of the Iranian Physical Society* (2002).
69. "Screening at doped nanotube junctions beyond linear response"
A. A. Farajian, K. Esfarjani and M. Mikami; *Phys. Rev. B* **65**, 165415 (2002).
70. "Statics and Dynamics of Phase Segregation in Multicomponent Fermion Gas"
K. Esfarjani, S. T. Chui, V. Kumar, and Y. Kawazoe; *Eur. Phys. J. D* **21**, 181 (2002).
71. "Electron-interaction effects on transport characteristics of nanotubes"
A.A. Farajian, K. Esfarjani, H. Mizuseki, and Y. Kawazoe; *Physica B*, **323**, 242 (2002).

72. "Electronic properties of magnetically doped nanotubes"
K. Esfarjani, Z. Chen and Y. Kawazoe; *Bull. Mater. Sci.*, **26**, 1, (2003).
73. "Effect of disorder and external potential on transmission and I-V characteristics of a quantum dot"
H. Cheraghchi and K. Esfarjani; *Proceedings of the Condensed Matter workshop, IASBS, Zanjan, Iran* (April 2003).
74. "First-principle calculation of electronic properties at junctions"
A. A. Shokri and K. Esfarjani; *Proceedings of the Condensed Matter workshop, IASBS, Zanjan, Iran* (April 2003).
75. "Spin excitations in a magnetic quantum dot"
K. Esfarjani and M. R. Mozaffari; *Proceedings of the Condensed Matter workshop, IASBS, Zanjan, Iran* (April 2003).
76. "Magnetic properties and evolution of vortex state in a quantum dot"
H. Haghgi and K. Esfarjani; *Proceedings of the Iranian Physical Society Meeting* (2003).
77. "A simple model to describe spin and charge couplings of an impurity in the electron gas"
A. A. Shokri and K. Esfarjani; *Proceedings of the Iranian Physical Society Meeting* (2003).
78. "Effect of co-polymerization on the spectrum and transmission properties in a quantum wire; a tight binding study"
M. Mardaani and K. Esfarjani; *Proceedings of the Iranian Physical Society Meeting* (2003).
79. "Oscillator strength calculations in color centers of diamond and the role of spin"
M. Heydari Saani, M. A. Vesaghi, and K. Esfarjani; *Eur. Phys. J. B* **39**, 441 (2004).
80. "Details of a theoretical model for electronic structure of diamond vacancies"
M. Heydari Saani, M. A. Vesaghi, K. Esfarjani and A. Shafiekhani; *Diamond and Related Materials*(DIAMAT) **13**, 2125 (2004).
81. "Some analytical results in phase coherent transport in quantum wires"
M. Mardaani, K. Esfarjani; *Physica E* **25**, 119 (2004).
82. "Calculation of charge and spin response in a polarized electron gas"
A. A. Shokri and K. Esfarjani; *Proceedings of the Condensed Matter workshop, IASBS, Zanjan, Iran* (April 2004).
83. "Effect of spin polarization on transport in a quantum wire"
A. A. Shokri and K. Esfarjani; *Proceedings of the Condensed Matter workshop, IASBS, Zanjan, Iran* (April 2004).
84. "Thermionic cooling in semiconductor junctions by Monte Carlo method"
M. Zebarjadi and K. Esfarjani; *Proceedings of the Condensed Matter workshop, IASBS, Zanjan, Iran* (April 2004).

85. "Nonlinear charging, and transport times in doped nanotube junctions"
K. Esfarjani, Amir A. Farajian, Siu Tat Chui and Yoshiyuki Kawazoe; J. Phys. Soc. Jap. **74**, 515 (2005).
86. "Lattice relaxation in many-electron states of the diamond vacancy"
M. Heydari Saani, M. A. Vesaghi, K. Esfarjani, T. Ghods Elahi, M. Saiari, H. Hashemi and N. Gorjizadeh; Phys. Rev. B **71**, 035202 (2005).
87. "Coherent conductance in an alternating dot: Exact results"
M. Mardaani, K. Esfarjani; Physica E. **27**, 227 (2005).
88. "Properties of charge and magnetic impurities in a spin-polarized electron gas: A semiclassical approach"
A. A. Shokri and K. Esfarjani; Physica E **28**, 313 (2005).
89. "Spin filtering and spin diode devices in quantum wire systems"
A. A. Shokri, M. Mardaani and K. Esfarjani; Physica E **27** 325, (2005).
90. "Analytical results on coherent conductance in a general periodic dot: Transfer matrix method"
M. Mardaani, A. A. Shokri and K. Esfarjani; Physica E **28**, 150 (2005).
91. "Analytical results on ballistic transport in a periodic molecular wire"
M. Mardaani, K. Esfarjani; Chem. Phys. **317**, 43 (2005).
92. "Molecular Dynamics of single wall carbon nanotube growth on nickel surface"
K. Esfarjani, Narjes, Gorjizadeh; to appear in Computational Materials Science (August 2005).
93. "Localization-delocalization transition in a one one-dimensional system with long-range correlated off-diagonal disorder"
H. Cheraghchi, S. M. Fazeli, and K. Esfarjani; Phys. Rev. B **72**, 174207 (2005).
94. "Thermoelectric properties of a nanocontact"
K. Esfarjani, M. Zebarjadi, A. Shakouri, and Y. Kawazoe; to appear in Phys. Rev. B (2006).