Publications

Amir A. Farajian

BOOK CHAPTERS

5 Field emission properties of carbon nanotubes from first-principles calculations,
M. Khazaei, A. A. Farajian, and Y. Kawazoe,
in **DFT calculations on fullerenes and carbon nanotubes**, *Edited by V. A. Basiuk and S. Irle,* (Research Signpost Publishers, in print).

4 Green's Function Formulation of Electronic Transport at Nanoscale,
A. A. Farajian, O. V. Pupysheva, B. I. Yakobson, and Y. Kawazoe,
in **Nano- and Micromaterials (Series on Advances in Materials Research)**, *Edited by K. Ohno, M. Tanaka, J. Takeda, and Y. Kawazoe,* (Springer-Verlag, Berlin, 2008).

3 Calculating transport properties of nanometer-scale systems: Nanodevice applications of carbon nanotubes and organic molecules,
A. A. Farajian, R. V. Belosludov, O. V. Pupysheva, H. Mizuseki, and Y. Kawazoe,
in **Nanostructures — Fabrication and Analysis**, *Edited by H. Nejo,* (Springer-Verlag, Berlin, 2007).

2 Electron transport in nanostructured systems — Ab initio study,
Y. Kawazoe, H. Mizuseki, R. Belosludov, A. Farajian,
in **Handbook of Theoretical and Computational Nanotechnology, Volume 10: Nanodevice Modeling and Nanoelectronics**, *Edited by M. Rieth and W. Schommers,* (American Scientific Publishers, 2006).

1 Electronic, transport and mechanical properties of carbon nanotubes,
K. Esfarjani, A. A. Farajian, Y. Hashi, and Y. Kawazoe,
in **Clusters and Nanomaterials: Theory and Experiment**, *Edited by Y. Kawazoe, T. Kondow, and K. Ohno,* (Springer-Verlag, Berlin, 2002).

REFEREED JOURNALS

51 The effects of defects on the conductance of graphene nanoribbons,
N. Gorjizadeh, A. A. Farajian, and Y. Kawazoe,
Nanotechnology **20**, 015201 (2009).

50 Spin and band-gap engineering in doped graphene nanoribbons,
N. Gorjizadeh, A. A. Farajian, K. Esfarjani, and Y. Kawazoe,
Phys. Rev. B **78**, 155427 (2008).

49 Polarization, energetics and electrorheology in nanotube suspensions under an applied electric field: An exact numerical approach,
A. A. Farajian, O. V. Pupysheva, H. K. Schmidt, and B. I. Yakobson,
Phys. Rev. B **77**, 205432 (2008).

48 Fullerene nanocage capacity for hydrogen storage,
O. V. Pupysheva, A. A. Farajian, and B. I. Yakobson,
Nano Lett. **8**, 767 (2008).

47 Electron transport of nanotube-based gas sensors: An ab initio study,
A. Sadrzadeh, A. A. Farajian, and B. I. Yakobson,
Appl. Phys. Lett. **92**, 022103 (2008).

46 Switching and negative differential resistance in a single-molecule transistor: Emergence of fixed and shifting states with molecular length,
A. A. Farajian, R. V. Belosludov, H. Mizuseki, Y. Kawazoe, T. Hashizume, and B. I. Yakobson,
J. Chem. Phys. **127**, 024901 (2007).

45 Field emission signature of pentagons at carbon nanotube caps,
M. Khazaei, K. A. Dean, A. A. Farajian, and Y. Kawazoe,
J. Phys. Chem. C **111**, 6690 (2007).

44 Electronic and transport properties of bismuth nanolines for applications in molecular electronics,
R. V. Belosludov, A. A. Farajian, H. Mizuseki, K. Miki, and Y. Kawazoe,
Phys. Rev. B **75**, 113411 (2007).

43 Transition between N- and Z-shaped current-voltage characteristics in semiconductor multiple-quantum-well structures,
O. V. Pupysheva, A. V. Dmitriev, A. A. Farajian, H. Mizuseki, and Y. Kawazoe,
J. Appl. Phys. **100**, 033718 (2006).

42 Theoretical study of conductance properties of metallocene,
T. Uehara, N. Igarashi, R. V. Belosludov, A. A. Farajian, H. Mizuseki, and Y. Kawazoe,
J. Jap. Inst. Met. **70**, 478 (2006).

41 Electronic and transport properties of ferrocene: Theoretical study,
T. Uehara, R. V. Belosludov, A. A. Farajian, H. Mizuseki, and Y. Kawazoe,
Jap. J. Appl. Phys. **45**, 3768 (2006).

40 Realization of molecular interconnection for molecular electronics: Theoretical aspects,
R. V. Belosludov, A. A. Farajian, Y. Kikuchi, H. Mizuseki, and Y. Kawazoe,
Comp. Mat. Sci. **36**, 130 (2006).

39 Cs doping effects on electronic structure of thin nanotubes,
M. Khazaei, A. A. Farajian, H. Mizuseki, and Y. Kawazoe,
Comp. Mat. Sci. **36**, 152 (2006).

38 Interaction of single-walled carbon nanotubes with alkylamines: An ab initio study,
O. V. Pupysheva, A. A. Farajian, H. Nejo, H. Mizuseki, and Y. Kawazoe,
Thin Solid Films **499**, 256 (2006).

37 A general-purpose approach for calculating transport in contact-molecule-contact systems: TARABORD implementation and application to a polythiophene-based nanodevice,
A. A. Farajian, R. V. Belosludov, H. Mizuseki, and Y. Kawazoe,
Thin Solid Films **499**, 269 (2006).

36 Theoretical study on junctions in porphyrin oligomers for nanoscale devices,
H. Mizuseki, R. V. Belosludov, A. A. Farajian, N. Igarashi, and Y. Kawazoe,
Mat. Sci. Eng. C **25**, 718 (2005).

35 An ab initio study of single-walled nanotubes bombarded with 50-150 eV Cs^+ ions,
M. Khazaei, A. A. Farajian, H. Mizuseki, and Y. Kawazoe,
Chem. Phys. Lett. **415**, 34 (2005).

34 Field emission patterns from first-principles electronic structures: Application to pristine and cesium-doped carbon nanotubes,
M. Khazaei, A. A. Farajian, and Y. Kawazoe,
Phys. Rev. Lett. **95**, 177602 (2005).

33 Electronic and transport properties of doped organic molecules for molecular wire applications,
R. V. Belosludov, A. A. Farajian, H. Baba, H. Mizuseki, and Y. Kawazoe,
Jpn. J. Appl. Phys. **44**, 2823 (2005).

32 Nonlinear charging and transport times in doped nanotubes junctions,
K. Esfarjani, A. A. Farajian, Y. Kawazoe, and S. T. Chui,
J. Phys. Soc. Jpn. **74**, 515 (2005).

31 Structure and electronic properties of metal di-(4-thiophenyl)-porphyrin,
Y. Kikuchi, R. V. Belosludov, H. Baba, A. A. Farajian, H. Mizuseki, and Y. Kawazoe,
Molecular Simulation **30**, 929 (2004).

30 Dynamical criteria for Cs-ion insertion and adsorption at cap and stem of carbon nanotubes: Ab initio study and comparison with experiment,
M. Khazaei, A. A. Farajian, G.-H. Jeong, H. Mizuseki, T. Hirata, R. Hatakeyama, and Y. Kawazoe,
J. Phys. Chem. B **108**, 15529 (2004).

29 Nanoswitch based on nanotubes: Bent-nanotubes transport,
A. A. Farajian, B. I. Yakobson, H. Mizuseki, and Y. Kawazoe,
Intl. J. Nanoscience **3**, 131 (2004).

28 Electron transport in molecular enamel wires,
R. V. Belosludov, A. A. Farajian, H. Mizuseki, K. Ichinoseki, and Y. Kawazoe,
Jpn. J. Appl. Phys. **43**, 2061 (2004).

27 Electronic transport properties of a metal-semiconductor carbon nanotube heterojunction,
A. A. Farajian, H. Mizuseki, and Y. Kawazoe,
Physica E **22**, 675 (2004).

26 Stable geometries and magnetic properties of single-walled carbon nanotubes with 3d transition metals: A first-principle study,
Y. Yagi, T. M. Briere, M. H. F. Sluiter, V. Kumar, A. A. Farajian, and Y. Kawazoe,
Phys. Rev. B **69**, 075414 (2004).

25 Molecular orbital analysis of frontier orbitals for molecular electronics: A case study of unimolecular rectifier and photovoltaic cell,
H. Mizuseki, R. V. Belosludov, A. A. Farajian, N. Igarashi, J.-T. Wang, H. Chen, C. Majumder, S. Miura, and Y. Kawazoe,
Sci. Technol. Adv. Mater. **4**, 377 (2003).

24 Theoretical study of molecular enamel wire based on polythiophene-cyclodextrin inclusion complexes,
R. V. Belosludov, H. Sato, A. A. Farajian, H. Mizuseki, and Y. Kawazoe,
Molecular Crystals and Liquid Crystals **406**, 195 (2003).

23 Theoretical study of donor-spacer-acceptor structure molecule for stable molecular rectifier,
H. Mizuseki, K. Niimura, C. Majumder, R. V. Belosludov, A. A. Farajian, and Y. Kawazoe,
Molecular Crystals and Liquid Crystals **406**, 205 (2003).

22 Genetic algorithm approach to aromatic molecules for nanoscale device,
H. Mizuseki, N. Igarashi, R. V. Belosludov, A. A. Farajian, and Y. Kawazoe,
Mater. Sci. Eng. C **23**, 807 (2003).

21 Cesium encapsulation in single-walled carbon nanotubes via plasma ion irradiation: Application to junction formation and ab initio investigation,
G. -H. Jeong, A. A. Farajian, R. Hatakeyama, T. Hirata, T. Yaguchi, K. Tohji, H. Mizuseki, and Y. Kawazoe,
Phys. Rev. B **68**, 075410 (2003).

20 Theoretical study of insulated wires based on polymer chains encapsulated in molecular nanotubes,
R. V. Belosludov, H. Sato, A. A. Farajian, H. Mizuseki, and Y. Kawazoe,
Thin Solid Films **438-439**, 80 (2003).

19 Theoretical study of a donor-spacer-acceptor structure molecule for use as a stable molecular rectifier: Geometric and electronic structures,
H. Mizuseki, N. Igarashi, C. Majumder, R. V. Belosludov, A. A. Farajian, and Y. Kawazoe,
Thin Solid Films **438-439**, 235 (2003).

18 Encapsulation of cesium inside single-walled carbon nanotubes by plasma-ion irradiation method,
G.-H. Jeong, A. A. Farajian, T. Hirata, R. Hatakeyama, K. Tohji, T. M. Briere, H. Mizuseki, and Y. Kawazoe,
Thin Solid Films **435**, 307 (2003).

17 Theoretical study of phthalocyanine-fullerene complex for a high efficiency photovoltaic device using ab initio electronic structure calculation,
H. Mizuseki, N. Igarashi, R. V. Belosludov, A. A. Farajian, and Y. Kawazoe,
Synthetic Metals **138**, 281 (2003).

16 Electronic transport through bent carbon nanotubes: Nanoelectromechanical sensors and switches,
A. A. Farajian, B. I. Yakobson, H. Mizuseki, and Y. Kawazoe,
Phys. Rev. B **67**, 205423 (2003).

15 Electronic transport through benzene molecule: Effect of gold contacts,
A. A. Farajian, R. V. Belosludov, H. Mizuseki, and Y. Kawazoe,
Physica E **18**, 253 (2003).

14 Molecular enamel wires for electronic devices: Theoretical study,
R. V. Belosludov, H. Sato, A. A. Farajian, H. Mizuseki, K. Ichinoseki, and Y. Kawazoe,
Jpn. J. Appl. Phys. **42**, 2492 (2003).

13 Theoretical study of chlorin-fullerene supramolecular complexes for photovoltaic devices,
H. Mizuseki, N. Igarashi, R. V. Belosludov, A. A. Farajian, and Y. Kawazoe,
Jpn. J. Appl. Phys. **42**, 2503 (2003).

12 Electron-interaction effects on transport characteristics of nanotubes,
A. A. Farajian, K. Esfarjani, H. Mizuseki, and Y. Kawazoe,
Physica B **323**, 242 (2002).

11 Screening at doped nanotube junctions beyond linear response,
A. A. Farajian, K. Esfarjani, and M. Mikami,
Phys. Rev. B **65**, 165415 (2002).

10 Transport properties of a nanotube-based transistor,
K. Esfarjani, A. A. Farajian, F. Ebrahimi, and Y. Kawazoe,
Eur. Phys. J. D **16**, 353 (2001).

9 Electronic and mechanical properties of C_{60}-doped nanotubes,
A. A. Farajian and M. Mikami,
J. Phys.: Condens. Matter **13**, 8049 (2001).

8 Ring closure in dioxin formation process: an ab initio molecular dynamics study,
A. A. Farajian, M. Mikami, P. Ordejon, and K. Tanabe,
J. Chem. Phys. **115**, 6401 (2001).

7 Why the all-electron full-potential approach is suitable for calculations on fullerenes and nanotubes?
Y. Kawazoe, K. Ohno, K. Esfarjani, Y. Maruyama, K. Shiga, and A. Farajian,
J. Mol. Graphics and Modelling **19**, 270 (2001).

6 Localized basis set optimization,
K. Esfarjani, A. A. Farajian, and Y. Kawazoe,
Comp. Mat. Sci. **15**, 351 (1999).

5 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).

4 Nonlinear coherent transport through doped nanotube junctions,
A. A. Farajian, K. Esfarjani, and Y. Kawazoe,
Phys. Rev. Lett. **82**, 5084 (1999).

3 The three-fermion problem in two and three dimensions; a unified variational approach,
A. A. Farajian, K. Esfarjani, and Y. Kawazoe,
J. Phys. B: At. Mol. Opt. Phys. **32**, 749 (1999).

2 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).

1 Penetration depth in anyon superconductivity on torus,
A. A. Farajian and A. A. Babaei Brojeny,
Mod. Phys. Lett. B **11**, 1255 (1997).