

Publications
AMIR A. FARAJIAN

REFEREED JOURNALS

- 67 Porosity effects on oxidation of ultra high temperature ceramics,
A. A. Farajian, M. B. Ruggles-Wrenn, and A. J. DeGregoria,
Journal of Materials Engineering and Performance, accepted.
- 66 *Ab initio* molecular dynamics of pipe diffusion in fcc Ni beyond transition state theory,
L. J. Wirth, C. Woodward, and A. A. Farajian,
Acta Materialia **222**, 117357 (2022).
- 65 Density functional study of self-diffusion along an isolated screw dislocation in fcc Ni,
L. J. Wirth, A. A. Farajian and C. Woodward,
Phys. Rev. Materials **3**, 033605 (2019).
- 64 Multiscale molecular thermodynamics of graphene-oxide liquid-phase exfoliation,
A. A. Farajian, R. Mortezaee, T. H. Osborn, O. V. Pupyshcheva, M. Wang, A. Zhamu and
B. Z. Jang,
Phys. Chem. Chem. Phys. **21**, 1761 (2019).
- 63 Systematic enhancement of thermoelectric figure of merit in edge-engineered nanoribbons,
L. J. Wirth and A. A. Farajian,
J. Phys. Chem. C **122**, 8843 (2018).
- 62 Resilience of thermal conductance in defected graphene, silicene, and boron nitride nanoribbons,
L. J. Wirth, T. H. Osborn and A. A. Farajian,
Appl. Phys. Lett. **109**, 173102 (2016).
- 61 Silicene nanoribbons as carbon monoxide nanosensors with molecular resolution,
T. H. Osborn and A. A. Farajian,
Nano Research **7**, 945 (2014).
- 60 *Ab initio* assessment of graphene nanoribbons reactivity for molecule adsorption and conductance modulation: nitrogen dioxide nanosensor,
K. K. Paulla, A. J. Hassan, C. R. Knick, and A. A. Farajian,
RSC Adv. **4**, 2346 (2014).
- 59 Concentration effects of carbon oxides on sensing by graphene nanoribbons:
Ab initio modeling,
K. K. Paulla and A. A. Farajian,
J. Phys. Chem. C **117**, 12815 (2013).
- 58 Stacking stability, emergence of magnetization and electromechanical nanosensing in bilayer graphene nanoribbons,
K. K. Paulla and A. A. Farajian,
J. Phys.: Condens. Matter **25**, 115303 (2013).
- 57 Stability of lithiated silicene from first principles,
T. H. Osborn and A. A. Farajian,
J. Phys. Chem. C **116**, 22916 (2012).
- 56 *Ab initio* simulations of silicene hydrogenation,
T. H. Osborn, A. A. Farajian, O. V. Pupyshcheva, R. S. Aga, and L. C. Lew Yan Voon,
Chem. Phys. Lett. **511**, 101 (2011).
- 55 Non-coherent transport in carbon chains,
N. Gorjizadeh, A. A. Farajian, and Y. Kawazoe,
J. Phys.: Condens. Matter. **23**, 075301 (2011).

- 54 Modeling direct exfoliation of nanoscale graphene platelets,
O. V. Pupyshva, A. A. Farajian, C. R. Knick, A. Zhamu, and B. Z. Jang,
J. Phys. Chem. C **114**, 21083 (2010).
- 53 Carbon nanotubes oscillation under electric field,
M. Khazaei, A. A. Farajian, S. U. Lee, R. V. Belosludov, and Y. Kawazoe,
Jpn. J. Appl. Phys. **49**, 115103 (2010).
- 52 Hydrogen compounds of group-IV nanosheets,
L. C. Lew Yan Voon, E. Sandberg, R. S. Aga, and A. A. Farajian,
Appl. Phys. Lett. **97**, 163114 (2010).
- 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. Pupyshva, H. K. Schmidt, and B. I. Yakobson,
Phys. Rev. B **77**, 205432 (2008).
- 48 Fullerene nanocage capacity for hydrogen storage,
O. V. Pupyshva, 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. Pupyshva, 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. Jpn. 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,
Jpn. 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. Pupyshova, 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 chlorine-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 C₆₀-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).

BOOK CHAPTERS

- 6 Electronic and transport properties of defected graphene nanoribbons,
N. Gorjizadeh, Y. Kawazoe, and A. A. Farajian
in **Physics and Applications of Graphene - Theory**, Edited by *S. Mikhailov*, (InTech Publishers, 2011).
- 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, 2008).
- 4 Green's Function Formulation of Electronic Transport at Nanoscale,
A. A. Farajian, O. V. Pupyshcheva, 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. Pupyshcheva, 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).