

# Curriculum Vitae

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## EDUCATION

- Ph. D. in Physics (advisor: Prof. Jisoon Ihm), Department of Physics, Seoul National University, Seoul, Korea, 2000
- M.S. in Physics, Department of Physics, Seoul National University, Seoul, Korea, 1994
- B.S. in Physics, Department of Physics, Seoul National University, Seoul, Korea, 1992

## EXPERIENCE

- Professor, School of Computational Sciences, Korea Institute for Advanced Study, Seoul, Korea, 2003 - present
- Miller Research Fellow (advisors: Profs. Steven G. Louie and Marvin L. Cohen), Department of Physics, University of California, Berkeley, USA, 2000 - 2003
- Postdoctoral Researcher, Center for Strongly Correlated Materials Research, Seoul National University, Seoul, Korea, 2000

## ACADEMIC HONORS AND AWARDS

- Miller Research Fellowship, University of California, Berkeley, 2000 – 2003
- An Honor Prize, Graduate Student Research Award, Physics Research Division, Seoul National University, 2000
- Best Graduate Student Fellowship, Development Foundation, Seoul National University, 1994

– 1996

- Graduate Student Scholarship, Seoul National University, 1992 - 1994

## RESEARCH INTERESTS

- First-principles study of electronic transport in nanostructures such as carbon nanotubes and molecular electronic devices.
- Theoretical investigation of superconducting properties of novel superconductors on the basis of first-principles calculation.
- *Ab-initio* calculation of physical properties of solids and molecules including crystal structures, electronic structures, and vibrational spectra.

## RESEARCH ACCOMPLISHMENTS

- **Superconducting mechanism of MgB<sub>2</sub>**: First-principles investigation of MgB<sub>2</sub> including the electronic structure, phonon spectra, electron-phonon interactions, superconducting transition temperature, isotope effects, structure of the superconducting energy gap on the Fermi surface, quasi-particle excitation spectra, and specific heat using the anisotropic Eliashberg formalism.
- **Structure and Electronic Structure of C<sub>60</sub> Monolayers**: First-principles study of the atomic geometries and electronic structures of C<sub>60</sub> monolayers on metal surfaces for the comparison with the experimental results of high-resolution angle-resolved photoemission spectroscopy.
- **Electronic Structure of Carbon Nanotube Junctions**: Calculation of the local density of states in carbon nanotube intramolecular junctions for the analysis of scanning tunneling spectroscopic data.
- **First-principles Method for the Calculation of Conductance in Quantum Wires**: Development of computational formalism for the conductance of atomic wires based on the *ab initio* nonlocal pseudopotential method.
- **Electronic Transport in Carbon Nanotubes with Defects**: First-principles calculation of the conductance of carbon nanotubes with substitutional boron and nitrogen impurities; pentagon-heptagon-pair defects; and carbon vacancies. Analytic calculation of conductance of armchair carbon nanotubes with defects within a simple tight-binding model.
- **Crossed Carbon Nanotube Junctions**: First-principles calculation of conductance of crossed metallic carbon nanotube junctions as a function of applied forces.

- **Electronic Structure of Carbon Nanotube Ropes:** Prediction of pseudogap opening by broken symmetry in the electronic structure of bundles of armchair metallic carbon nanotubes.
- **Excitonic Tunneling Rate in  $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$  Double Quantum Wells:** Numerical calculation of tunneling probability through a three-dimensional percolative barrier as a model for excitonic tunneling through an  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  barrier in  $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$  double quantum wells.

## PUBLICATIONS

- V. Brouet, W. L. Yang, X. J. Zhou, H. J. Choi, S. G. Louie, M. L. Cohen, A. Goldoni, F. Parmigiani, Z. Hussain, Z.-X. Shen, "Orientation-dependent  $\text{C}_{60}$  electronic structures revealed by angle-resolved photoemission", *Physical Review Letters* **93**, 197601-1 – 197601-4 (2004).
- M. Ishigami, H. J. Choi, S. Aloni, S. G. Louie, M. L. Cohen, A. Zettl, "Identifying defects in nanoscale materials", *Physical Review Letters* **93**, 196803-1 – 196803-4 (2004).
- H. J. Choi, D. Roundy, H. Sun, M. L. Cohen, S. G. Louie, "Reply to 'Comment on 'First-principles calculation of the superconducting transition in  $\text{MgB}_2$  within the anisotropic Eliashberg formalism' " ", *Physical Review B* **69**, 056502-1 – 056502-1 (2004).
- W. L. Yang, V. Brouet, X. J. Zhou, H. J. Choi, S. G. Louie, M. L. Cohen, S. A. Kellar, P. V. Bogdanov, A. Lanzara, A. Goldoni, F. Parmigiani, Z. Hussain, Z.-X. Shen, "Band structure and Fermi surface of electron-doped  $\text{C}_{60}$  monolayers", *Science* **300**, 303-307 (2003).
- H. J. Choi, M. L. Cohen, S. G. Louie, "Anisotropic Eliashberg theory of  $\text{MgB}_2$ : Tc, isotope effects, superconducting energy gaps, quasiparticles, and specific heat", *Physica C* **385**, 66-74 (2003) (invited paper for special issue on  $\text{MgB}_2$ ).
- H. J. Choi, D. Roundy, H. Sun, M. L. Cohen, S. G. Louie, "The origin of the anomalous superconducting properties of  $\text{MgB}_2$ ", *Nature* **418**, 758-760 (2002).
- H. J. Choi, D. Roundy, H. Sun, M. L. Cohen, S. G. Louie, "First-principles calculation of the superconducting transition in  $\text{MgB}_2$  within the anisotropic Eliashberg formalism", *Physical Review B* **66**, 020513-1 – 020513-4 (2002).
- Y.-G. Yoon, M. S. C. Mazzoni, H. J. Choi, J. Ihm, S. G. Louie, "Structural deformation and intertube conductance of crossed carbon nanotube junctions", *Physical Review Letters* **86**, 688-691 (2001).
- M. S. Fuhrer, J. Nygard, L. Shih, M. Forero, Y.-G. Yoon, M. S. C. Mazzoni, H. J. Choi, J. Ihm, S. G. Louie, A. Zettl, P. L. McEuen, "Crossed nanotube junctions", *Science* **288**, 494-497 (2000).

- H. J. Choi, J. Ihm, S. G. Louie, M. L. Cohen, “Defects, quasi-bound states, and quantum conductance in metallic carbon nanotubes”, *Physical Review Letters* **84**, 2917-2920 (2000).
- H. J. Choi, J. Ihm, Y.-G. Yoon, S. G. Louie, “Possible explanation for the conductance of a single quantum unit in metallic carbon nanotubes”, *Physical Review B* **60**, R14009-14011 (1999).
- P. Delaney, H. J. Choi, J. Ihm, S. G. Louie, M. L. Cohen, “Broken symmetry and pseudogaps in ropes of carbon nanotubes”, *Physical Review B* **60**, 7899-7904 (1999).
- H. J. Choi, J. Ihm, “Exact solutions to the tight-binding model for the conductance of carbon nanotubes”, *Solid State Communications* **111**, 385-390 (1999).
- H. J. Choi, J. Ihm, “Ab initio pseudopotential method for the calculation of conductance in quantum wires”, *Physical Review B* **59**, 2267-2275 (1999).
- P. Delaney, H. J. Choi, J. Ihm, S. G. Louie, M. L. Cohen, “Broken symmetry and pseudogaps in ropes of carbon nanotubes”, *Nature* **391**, 466-468 (1998).
- D. S. Kim, H. S. Ko, Y. M. Kim, S. J. Rhee, S. C. Hohng, Y. H. Yee, W. S. Kim, J. C. Woo, H. J. Choi, J. Ihm, D. H. Woo, K. N. Kang, “Percolation of carriers through low potential channels in thick  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  ( $x < 0.35$ ) barriers”, *Physical Review B* **54**, 14580-14588 (1996).
- D. S. Kim, H. S. Ko, Y. M. Kim, S. J. Rhee, S. C. Hong, Y. H. Yee, D. S. Yee, J. C. Woo, H. J. Choi, J. Ihm, D. H. Woo, K. N. Kang, “Thick  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  - an intrinsically percolating barrier owing to its microscopic structural inhomogeneity”, *Applied Physics Letters* **69**, 2513-2515 (1996).
- D. S. Kim, H. S. Ko, Y. M. Kim, S. J. Rhee, S. C. Hong, Y. H. Yee, W. S. Kim, J. C. Woo, H. J. Choi, J. Ihm, D. H. Woo, K. N. Kang, “Anomalous real-space charge-transfer through thick barriers in  $\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}$  as a symmetrical double- quantum wells -  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  as a percolating barrier”, *Solid State Communications* **100**, 231-235 (1996).
- D. S. Kim, H. S. Ko, Y. S. Lim, Y. M. Kim, J. S. Lee, S. J. Rhee, W. S. Kim, S. C. Hong, Y. H. Yee, J. S. Khim, J. M. Jung, S. Huhr, J. H. Lee, J. S. Chang, B. D. Choe, J. C. Woo, P. H. Song, H. J. Choi, S. H. Jhi, J. Ihm, E. J. Shin, D. Kim, D. H. Woo, K. N. Kang, J. J. Song, “Going beyond the mean-field approximations of alloys and alloy superlattices - a few puzzles solved”, *Journal of the Optical society of America B-Optical Physics* **13**, 1210-1223 (1996).
- D. S. Kim, H. S. Ko, Y. M. Kim, S. J. Rhee, W. S. Kim, J. C. Woo, H. J. Choi, J. Ihm, D. H. Woo, K. N. Kang, “Anomalously large Stokes and anti-Stokes real-space charge-transfer between quantum-wells separated by thick alloy barriers - beyond the mean-field approach”, *Institute of Physics Conference Series* **145**, 855-860 (1996).

## **SEMINARS AND CONFERENCE PRESENTATIONS**

- H. J. Choi, "First-principles calculation of nonlinear electrical transport in nanostructures", Seminar, Chonnam National University, Kwangju, South Korea, 2004.
- H. J. Choi, S. G. Louie, M. L. Cohen, "Structures and electronic structures of  $K_3C_{60}$  monolayers", 7th Asian Workshop on First-Principles Electronic Structure Calculations, Tamkang University, Taipei, Taiwan, 2004.
- H. J. Choi, "First-principles simulation of electrical transport in nanostructures", Invited talk, Korean-German Science and Technology Forum, Seoul, South Korea, 2004.
- H. J. Choi, "Structures and electronic structures of potassium-doped  $C_{60}$  monolayers", Invited talk, Korea Supercomputing Workshop, KISTI, Taejon, South Korea, 2004.
- H. J. Choi, "Anisotropic Eliashberg theory of  $MgB_2$ ", Plenary talk, Korean Superconductivity Society Meeting, Yongpyong, South Korea, 2004.
- H. J. Choi, "Anisotropic Eliashberg theory of  $MgB_2$ ", Invited talk, Korean Physical Society, Spring Meeting, South Korea, 2004.
- H. J. Choi, M. L. Cohen, S. G. Louie, "First-principles scattering-state approach to nonlinear electrical transport in nanostructures", American Physical Society, March Meeting, Canada, 2004.
- J. B. Neaton, K. H. Khoo, H. J. Choi, S. G. Louie, "Nonlinear quantum transport through carbon nanostructures and molecules from first principles", American Physical Society, March Meeting, Canada, 2004.
- Y.-W. Son, H. J. Choi, S. G. Louie, M. L. Cohen, J. Ihm, "Theoretical study on nonequilibrium charge transport through single organic molecules", American Physical Society, March Meeting, Canada, 2004.
- H. J. Choi, "Anisotropic Eliashberg theory of  $MgB_2$ ", Invited talk, 8th APCTP Winter Workshop on Strongly Correlated Electron Systems, Phoenix Park, South Korea, 2004.
- H. J. Choi, "Quantum conductance in nanostructures", Special lecture, KIAS-SNU Physics Winter Camp, Korea Institute for Advanced Study, Seoul, South Korea, 2004.
- H. J. Choi, "Nonlinear electronic transport in nanostructures", Invited talk, 6<sup>th</sup> Asian Workshop on First-Principles Electronic Structure Calculations, Tsukuba, Japan, 2003.

- Y.-W. Son, H. J. Choi, J. Ihm, “Quantum conductance of defective carbon nanotubes under transverse electric field”, 6<sup>th</sup> Asian Workshop on First-Principles Electronic Structure Calculations, Tsukuba, Japan, 2003.
- Y.-W. Son, H. J. Choi, S. G. Louie, M. L. Cohen, J. Ihm, “Nonequilibrium charge transport through single organic molecules”, Korean Physical Society, Fall Meeting, Daegu, South Korea, 2003.
- Y.-W. Son, Y. Cho, W. Choi, C.-K. Lee, J. Ihm, H. J. Choi, “Quantum conductance of defective double-wall carbon nanotube under transverse electric field”, Korean Physical Society, Fall Meeting, Daegu, South Korea, 2003.
- H. J. Choi, “Multi-gap superconductivity in MgB<sub>2</sub>”, Seminar, Department of Physics, Pohang University of Science and Technology, Pohang, South Korea, 2003.
- H. J. Choi, “Superconductivity of MgB<sub>2</sub> from first principles”, Seminar, Quantum Photonic Science Research Center, Hanyang University, Seoul, South Korea, 2003.
- H. J. Choi, “Multi-gap superconductivity in MgB<sub>2</sub>”, Seminar, Department of Physics, Korea Advanced Institute of Science and Technology, Taejon, South Korea, 2003.
- H. J. Choi, “First-principles study of superconductivity in MgB<sub>2</sub>”, Special Condensed Matter Physics Seminar, Department of Physics, Sungkyunkwan University, Suwon, South Korea, 2003.
- H. J. Choi, “First-principles study of superconductivity in MgB<sub>2</sub>”, CTP seminar, Department of Physics, Seoul National University, Seoul, South Korea, 2003.
- H. J. Choi, “First-principles study of superconductivity in MgB<sub>2</sub>”, Seminar, Computational Sciences, Korea Institute for Advanced Study, Seoul, South Korea, 2003.
- H. J. Choi, “Physical understanding of the anomalous superconducting properties in MgB<sub>2</sub>”, Colloquium, Department of Physics, Yonsei University, Seoul, South Korea, 2003.
- H. J. Choi, “First-principles study of superconductivity in MgB<sub>2</sub>”, Special Condensed Matter Physics Seminar, Department of Physics, University of California, San Diego, California, USA, 2003.
- H. J. Choi, “Electronic conduction in nanostructures: first-principles study”, Solid State and Optics Seminar, Department of Applied Physics, Yale University, New Haven, Connecticut, USA, 2003.
- H. J. Choi, “Multi-gap superconductivity in MgB<sub>2</sub>”, Invited talk, American Physical Society, March Meeting, USA, 2003.

- H. J. Choi, “First-principles study of superconductivity in  $\text{MgB}_2$ ”, Special Seminar, Physics and Astronomy Department, University of British Columbia, Vancouver, Canada, 2003.
- H. J. Choi, “First-principles study of superconductivity in  $\text{MgB}_2$ ”, 290k Seminar, Department of Physics, University of California, Berkeley, California, USA, 2002.
- H. J. Choi, “Superconductivity of  $\text{MgB}_2$  from first principles”, Invited talk, Fourteenth Annual Workshop on Recent Developments in Electronic Structure Methods, Berkeley, California, USA, 2002.
- H. J. Choi, D. Roundy, H. Sun, M. L. Cohen, S. G. Louie, “First-principles study of the superconducting transition, superconducting energy gaps, low temperature specific heat, and quasiparticle spectra in  $\text{MgB}_2$ ”, American Physical Society, March Meeting, USA, 2002.
- H. J. Choi, “Superconductivity of  $\text{MgB}_2$  from first-principles”, Solid State and Optics Seminar, Department of Applied Physics, Yale University, New Haven, Connecticut, USA, 2002.
- H. J. Choi, J. Ihm, Y.-G. Yoon, S. G. Louie, M. L. Cohen, “Electronic transport and structure in carbon nanotube junctions”, International Workshop on the Science and Application of Nanotubes, Potsdam, Germany, 2001.
- H. J. Choi, J. Ihm, Y.-G. Yoon, S. G. Louie, M. L. Cohen, “Electronic transport in carbon nanotube junctions”, American Physical Society, March Meeting, USA, 2001.
- H. Sun, D. Roundy, H. J. Choi, S. G. Louie, M. L. Cohen, “First principle pseudopotential calculation of the pressure dependence of the electronic properties of  $\text{MgB}_2$ ”, American Physical Society, March Meeting, USA, 2001.
- D. Roundy, H. J. Choi, H. Sun, S. G. Louie, M. L. Cohen, “Ab initio calculations of the phonon frequencies, Gruneisen constants, and electron-phonon coupling in  $\text{MgB}_2$ ”, American Physical Society, March Meeting, USA, 2001.
- H. J. Choi, “The conductance of carbon nanotubes contacted with liquid metals”, Invited talk, Korean Physical Society, Spring Meeting, South Korea, 2000.
- H. J. Choi, J. Ihm, Y.-G. Yoon, S. G. Louie, “Contact resistance of carbon nanotubes and metals”, American Physical Society, March Meeting, USA, 2000.
- Y.-G. Yoon, M. Mazzoni, S. G. Louie, H. J. Choi, J. Ihm, “First-principles study of intertube conductance of crossed carbon nanotube junctions”, American Physical Society, March Meeting, USA, 2000.
- H. J. Choi, J. Ihm, “Contact resistance of carbon nanotubes and metals”, Invited talk, The 10<sup>th</sup> Symposium on Theoretical Solid State Physics, Taejon, South Korea, 2000.

- H. J. Choi, J. Ihm, “First-principles study of the effects of impurities and defects on the conductance of carbon nanotubes”, 2<sup>nd</sup> Korea-Japan Joint Workshop on Electronic Structure Calculations, Seoul, South Korea, 1999.
- J. H. Lee, H. J. Choi, J. Ihm, “Conductance of capped carbon nanotubes”, Korean Physical Society, Fall Meeting, South Korea, 1999.
- T. J. Sung, H. J. Choi, J. Ihm, “A numerical study on the magnetoresistance of carbon nanotubes in the weak localization regime”, Korean Physical Society, Fall Meeting, South Korea, 1999.
- H. J. Choi, J. Ihm, “Ab initio calculation for the conductance of carbon nanotubes with defects”, American Physical Society, March Meeting, USA, 1999.
- H. J. Choi, J. Ihm, “The effect of local defects on the conductance of the carbon nanotube”, International Workshop on Semiconductor Quantum Structures, Cheju, South Korea, 1998.
- H. J. Choi, J. Ihm, “The quantum conductance of the carbon nanotube with a local defect”, APCTP-ICTP Joint International Conference, Seoul, South Korea, 1998.
- P. Delany, S. G. Louie, M. L. Cohen, J. Ihm, H. J. Choi, “Pseudogap in ropes of (10,10) carbon nanotubes”, American Physical Society, March Meeting, USA, 1998.
- H. J. Choi, J. Ihm, “Short-range-order effect on the tunneling of the GaAs heavy hole in GaAs/Al<sub>x</sub>Ga<sub>1-x</sub>As/GaAs single barrier structures”, American Physical Society, March Meeting, USA, 1997.
- H. J. Choi, J. Ihm, “Short-range-order effect on the tunneling of the GaAs heavy hole in GaAs/Al<sub>x</sub>Ga<sub>1-x</sub>As/GaAs single barrier structures”, The 7<sup>th</sup> Symposium on Theoretical Solid State Physics, Taejon, South Korea, 1997.