

List of Publications — Jaejun Yu

1. "Synthesis and Magnetic Properties of the Multiferroic $[C(NH_2)_3]Cr(HCOO)_3$ Metal--Organic Framework: The Role of Spin--Orbit Coupling and Jahn-Teller Distortions," K. Yananose, E. R. Clark, P. J. Saines, P. Barone, A. Stroppa, and Jaejun Yu, *Inorganic Chemistry* 62, 17299 (2023).
doi: <https://doi.org/10.1021/acs.inorgchem.3c02557>
2. "Origin of morphotropic phase boundary in thin-film $Hf_0.5Zr_0.5O_2$ on the TiN electrode," I. Young Lee and Jaejun Yu, *Journal of Applied Physics* 134, 074102 (2023).
doi: <https://doi.org/10.1063/5.0159496>
3. "Efficient discovery of multiple minimum action pathways using Gaussian process," J. Shim, J. Lee, and Jaejun Yu, *Journal of Physics Communications* 7, 025004 (2023).
doi: <https://dx.doi.org/10.1088/2399-6528/acba83>
4. "Field-controlled quantum anomalous Hall effect in electron-doped $CrSiTe_3$ monolayer," S. Kang, S. Kang, H.-S. Kim, and Jaejun Yu, *npj 2D Materials and Applications* 7, 13 (2023).
doi: <https://doi.org/10.1038/s41699-023-00375-3>
5. "Activating magnetoelectric optical properties by twisting antiferromagnetic bilayers," K. Yananose, P. G. Radaelli, M. Cuoco, Jaejun Yu, and A. Stroppa, *Phys. Rev. B* 106, 184408 (2022).
doi: <https://doi.org/10.1103/PhysRevB.106.184408>
6. "Electronic structure and magnetic properties of transition metal Kagome metal-organic frameworks," S. Kang and Jaejun Yu, *Phys. Chem. Chem. Phys.* 24, 22168 (2022).
doi: <http://dx.doi.org/10.1039/D2CP02612K>
7. "Growth of bilayer MoTe₂ single crystals with strong non-linear Hall effect," T. Ma, H. Chen, K. Yananose, X. Zhou, L. Wang, R. Li, Z. Zhu, Z. Wu, Q.-H. Xu, Jaejun Yu, C. W. Qiu, A. Stroppa, and K. P. Loh, *Nature Communications* 13, 5465 (2022).
doi: <https://doi.org/10.1038/s41467-022-33201-3>
8. "Structure and disorder in MgSiO₃ glasses above megabar pressures via nuclear magnetic resonance: DFT calculations," S. K. Lee, J.-H. Parq, Y. S. Yi, S. Lee, H.-I. Kim, S.-M. Lee, and Jaejun Yu, *Journal of the American Ceramic Society* 105, 5151 (2022).
doi: <https://doi.org/10.1111/jace.18481>
9. "Band gap narrowing of TiO₂ nanoparticles: A passivated Co-doping approach for enhanced photocatalytic activity," S. Na-Phattalung, D. J. Harding, P. Pattanasattayavong, H. Kim, J. Lee, D.-W. Hwang, T. D. Chung, and Jaejun Yu, *Journal of Physics and Chemistry of Solids* 162, 110503 (2022).
doi: <https://doi.org/10.1016/j.jpcs.2021.110503>
10. "Chirality-induced spin texture switching in twisted bilayer graphene," K. Yananose, G. Cantele, P. Lucignano, S.-W. Cheong, Jaejun Yu, and A. Stroppa, *Phys. Rev. B* 104, 075407 (2021).
doi: <https://link.aps.org/doi/10.1103/PhysRevB.104.075407>
11. "Inevitable high density of oxygen vacancies at the surface of polar--nonpolar perovskite heterostructures LaAlO₃/SrTiO₃," Y. Li, X. Wei, and Jaejun Yu, *Journal of Applied Physics* 127, 205302 (2020).
doi: <https://doi.org/10.1063/1.5128080>
12. "Chern insulator with a nearly flat band in the metal-organic-framework-based Kagome lattice," S. Baidya, S. Kang, C. H. Kim, and Jaejun Yu, *Scientific Reports* 9, 13807 (2019).
doi: <https://doi.org/10.1038/s41598-019-50163-7>
13. "Superstructures of Se adsorbates on Au(111): Scanning tunneling microscopy and spectroscopy study," M. Lee, S. Kang, M. Oh, J. Chae, Jaejun Yu, and Y. Kuk, *Surface Science* 685, 19 (2019).
doi: <https://doi.org/10.1016/j.susc.2019.03.002>
14. "A Room-Temperature Ferroelectric Ferromagnet in a 1D Tetrahedral Chain Network," K. T. Kang, C. J. Roh, J. Lim, T. Min, J. H. Lee, K. Lee, T. Y. Lee, S. Kang, D. Seol, J. Kim, H. Ohta, A. Khare, S. Park,

- Y. Kim, S. C. Chae, Y. S. Oh, J. Lee, Jaejun Yu, J. S. Lee, and W. S. Choi, Advanced Materials 31, 1808104 (2019).
doi: <https://doi.org/10.1002/adma.201808104>
15. "Coulomb-interaction effect on the two-dimensional electronic structure of the van der Waals ferromagnet Cr₂Ge₂Te₆," M. Suzuki, B. Gao, K. Koshiishi, S. Nakata, K. Hagiwara, C. Lin, Y. X. Wan, H. Kumigashira, K. Ono, S. Kang, S. Kang, Jaejun Yu, M. Kobayashi, S.-W. Cheong, and A. Fujimori, Phys. Rev. B 99, 161401 (2019).
doi: <https://doi.org/10.1103/PhysRevB.99.161401>
16. "Effect of Coulomb Interactions on the Electronic and Magnetic Properties of Two-Dimensional CrSiTe₃ and CrGeTe₃ Materials," S. Kang, S. Kang, and J. Yu, Journal of Electronic Materials 48, 1441 (2019).
doi: <https://doi.org/10.1007/s11664-018-6601-2>
17. "Tunable magnetic topological insulating phases in monolayer CrI₃," S. Baidya, Jaejun Yu, and C. H. Kim, Phys. Rev. B 98, 155148 (2018).
doi: <https://doi.org/10.1103/PhysRevB.98.155148>
18. "Role of oxygen vacancy in the spin-state change and magnetic ordering in SrCoO_{3-δ}," J. Lim and Jaejun Yu, Phys. Rev. B 98, 085106 (2018).
doi: <https://doi.org/10.1103/PhysRevB.98.085106>
19. "Magnetic interactions in PdCrO₂ and their effects on its magnetic structure," M. D. Le, S. Jeon, A. I. Kolesnikov, D. J. Voneshen, A. S. Gibbs, J. S. Kim, J. Jeong, H.-J. Noh, C. Park, Jaejun Yu, T. G. Perring, and J.-G. Park, Phys. Rev. B 98, 024429 (2018).
doi: <https://doi.org/10.1103/PhysRevB.98.024429>
20. "Half-metallic ferromagnetism and metal--insulator transition in Sn-doped SrRuO₃ perovskite oxides", Namwook Kim, Rokyeon Kim, and Jaejun Yu, Journal of Magnetism and Magnetic Materials 460, 54 - 60 (2018.Aug 15).
doi: <https://doi.org/10.1016/j.jmmm.2018.03.034>
21. "Identification of F impurities in F-doped ZnO by synchrotron X-ray absorption near edge structures", Sutassana Na-Phattalung, Sukit Limpijumnong, Chul-Hee Min, Deok-Yong Cho, Seung-Ran Lee, Kookrin Char, and Jaejun Yu, Journal of Applied Physics 123, 161528 (2018.April).
doi: [10.1063/1.4997356](https://doi.org/10.1063/1.4997356)
22. "Band gap and mobility of epitaxial perovskite BaSn_{1-x}Hf_xO₃ thin films", Juyeon Shin, Jinyoung Lim, Taewoo Ha, Young Mo Kim, Chulkwon Park, Jaejun Yu, Jae Hoon Kim, and Kookrin Char, Phys. Rev. Materials 2, 021601 (2018.Feb).
doi: [10.1103/PhysRevMaterials.2.021601](https://doi.org/10.1103/PhysRevMaterials.2.021601)
23. "Graphene analogue in (111)-oriented BaBiO₃ bilayer heterostructures for topological electronics", Rokyeon Kim, Jaejun Yu, and Hosub Jin, Scientific Reports 8, 555 (2018.Jan).
doi: [10.1038/s41598-017-19090-3](https://doi.org/10.1038/s41598-017-19090-3)
24. "Magnetic states and intervalence charge transfer of Ti and Fe defects in α-Al₂O₃: The origin of the blue in sapphire", Sutassana Na-Phattalung, Sukit Limpijumnong, Jiraroj T-Thienprasert, and Jaejun Yu, Acta Materialia 143, 248 - 256 (2018.Jan). doi: <https://doi.org/10.1016/j.actamat.2017.10.006>
25. "Identification of F impurities in F-doped ZnO by synchrotron X-ray absorption near edge structures", Sutassana Na-Phattalung, Sukit Limpijumnong, Chul-Hee Min, Deok-Yong Cho, Seung-Ran Lee, Kookrin Char, and Jaejun Yu, Journal of Applied Physics 123, 161528 (2018). doi: [10.1063/1.4997356](https://doi.org/10.1063/1.4997356)
26. "High-k perovskite gate oxide BaHfO₃", Y.M. Kim, C. Park, T. Ha, U. Kim, N. Kim, J. Shin, Y. Kim, J. Yu, J.H. Kim, and K. Char, APL Materials 5, (2017.Jan). doi: [10.1063/1.4974864](https://doi.org/10.1063/1.4974864)
27. "Graphene as a flexible template for controlling magnetic interactions between metal atoms", Sungwoo Lee, Dongwook Kim, Alex W Robertson, Euijoon Yoon, Suklyun Hong, Jisoon Ihm,

- Jaejun Yu, Jamie H Warner, and Gun-Do Lee, Journal of Physics: Condensed Matter **29**, 085001 (2017.Jan). doi: <https://doi.org/10.1088/1361-648X/aa5167>
28. "Passivated co-doping approach to bandgap narrowing of titanium dioxide with enhanced photocatalytic activity", Sutassana Na Phattalung, Sukit Limpijumnong, and Jaejun Yu, Applied Catalysis B: Environmental **200**, 1 - 9 (2017.Jan). doi: <http://dx.doi.org/10.1016/j.apcatb.2016.06.054>
29. "Ab Initio Study of Elastic Properties of High-Pressure Polymorphs of CO₂ Phases II and V", Jae-Hyeon Park, Sung Keun Lee, Sang-Mook Lee, and Jaejun Yu, The Journal of Physical Chemistry C **120**, 23152 (2016.Sep). doi: <10.1021/acs.jpcc.6b07833>
30. "All-perovskite transparent high mobility field effect using epitaxial BaSnO₃ and LaInO₃", Useong Kim, Chulkwon Park, Taewoo Ha, Young Mo Kim, Namwook Kim, Chanjong Ju, Jisung Park, Jaejun Yu, Jae Hoon Kim, and Kookrin Char, APL Materials **3**, 036101 (2015.). doi: <http://dx.doi.org/10.1063/1.4913587>
31. "Dopant-site-dependent scattering by dislocations in epitaxial films of perovskite semiconductor BaSnO₃", Useong Kim, Chulkwon Park, Taewoo Ha, Rokyeon Kim, Hyo Sik Mun, Hoon Min Kim, Hyung Joon Kim, Tai Hoon Kim, Namwook Kim, Jaejun Yu, Kee Hoon Kim, Jae Hoon Kim, and Kookrin Char, APL Materials **2**, 056107 (2014.5). doi: <http://dx.doi.org/10.1063/1.4874895>
32. "Charge and magnetic states of rutile TiO₂ doped with Cr ions", Rokyeon Kim, Suyeon Cho, Won-Goo Park, Deok-Yong Cho, Se-Jung Oh, Romuald Saint-Martin, Patrick Berthet, Je-Geun Park, and Jaejun Yu, Journal of Physics: Condensed Matter **26**, 146003 (2014.3). doi: <http://dx.doi.org/10.1088/0953-8984/26/14/146003>
33. "Impact of vacancy clusters on characteristic resistance change of nonstoichiometric strontium titanate nano-film", Yong Su Kim, Jiyeon Kim, Moon Jee Yoon, Chang Hee Sohn, Shin Buhm Lee, Daesu Lee, Byung Chul Jeon, Hyang Keun Yoo, Tae Won Noh, Aaron Bostwick, Eli Rotenberg, Jaejun Yu, Sang Don Bu, and Bongjin Simon Mun, Applied Physics Letters **104**, 013501 (2014.Jan). doi: <http://dx.doi.org/10.1063/1.4860961>
34. "Enhanced upper critical fields in a new quasi-one-dimensional superconductor Nb₂Pd_xSe₅", Seunghyun Khim, Bumsung Lee, Ki-Young Choi, Byung-Gu Jeon, Dong Hyun Jang, Deepak Patil, Seema Patil, Rokyeon Kim, Eun Sang Choi, Seongsu Lee, Jaejun Yu, and Kee Hoon Kim, New Journal of Physics **15**, 123031 (2013.12). doi: <http://dx.doi.org/10.1088/1367-2630/15/12/123031>
35. "Large in-plane deformation of RuO₆ octahedron and ferromagnetism of bulk SrRuO₃", Sanghyun Lee, J R Zhang, S Torii, Seongil Choi, Deok-Yong Cho, T Kamiyama, Jaejun Yu, K A McEwen, and Je-Geun Park, Journal of Physics: Condensed Matter **25**, 465601 (2013.Oct). doi: <10.1088/0953-8984/25/46/465601>
36. "Indications of strong neutral impurity scattering in Ba(Sn,Sb)O₃ single crystals", Hyung Joon Kim, Jiyeon Kim, Tai Hoon Kim, Woong-Jhae Lee, Byung-Gu Jeon, Ju-Young Park, Woo Seok Choi, Da Woon Jeong, Suk Ho Lee, Jaejun Yu, Tae Won Noh, and Kee Hoon Kim, Phys. Rev. B **88**, 125204 (2013.Sep). doi: <10.1103/PhysRevB.88.125204>
37. "Mixing between $J_{\text{eff}}=1/2$ and 3/2 orbitals in Na₂IrO₃: A spectroscopic and density functional calculation study", C. H. Sohn, H.-S. Kim, T. F. Qi, D. W. Jeong, H. J. Park, H. K. Yoo, H. H. Kim, J.-Y. Kim, T. D. Kang, Deok-Yong Cho, G. Cao, J. Yu, S. J. Moon, and T. W. Noh, Phys. Rev. B **88**, 085125 (2013.Aug). doi: <10.1103/PhysRevB.88.085125>
38. "Temperature Evolution of Itinerant Ferromagnetism in SrRuO₃ Probed by Optical Spectroscopy", D. W. Jeong, Hong Chul Choi, Choong H. Kim, Seo Hyoung Chang, C. H. Sohn, H. J. Park, T. D. Kang, Deok-Yong Cho, S. H. Baek, C. B. Eom, J. H. Shim, Jaejun Yu, K. W. Kim, S. J. Moon, and T. W. Noh, Phys. Rev. Lett. **110**, 247202 (2013.Jun). doi: <10.1103/PhysRevLett.110.247202>
39. "Two-dimensional electron gas generated by La-doping at SrTiO₃(001) surface: A first-principles study", Yun Li and Jaejun Yu, AIP Advances **3**, 062116 (2013.June). doi: <10.1063/1.4811370>

40. "Modulation of electron carrier density at the n-type $\text{LaAlO}_3/\text{SrTiO}_3$ interface by water adsorption", Yun Li and Jaejun Yu, Journal of Physics: Condensed Matter **25**, 265004 (2013.June). doi: [10.1088/0953-8984/25/26/265004](https://doi.org/10.1088/0953-8984/25/26/265004)
41. "Collinear and noncollinear spin ground state of wurtzite CoO ", Myung Joon Han, Heung-Sik Kim, Dong Geun Kim, and Jaejun Yu, Phys. Rev. B **87**, 184432 (2013.May). doi: [10.1103/PhysRevB.87.184432](https://doi.org/10.1103/PhysRevB.87.184432)
42. "Strain-induced topological insulator phase and effective magnetic interactions in Li_2IrO_3 ", Heung-Sik Kim, Choong H. Kim, Hogyun Jeong, Hosub Jin, and Jaejun Yu, Phys. Rev. B **87**, 165117 (2013.Apr). doi: [10.1103/PhysRevB.87.165117](https://doi.org/10.1103/PhysRevB.87.165117)
43. "Geometric and electronic properties of porphyrin molecules on $\text{Au}(111)$ and NaCl surfaces", Seong Heon Kim, H.G. Jeong, S.J. Lim, U.D. Ham, Y.J. Song, Jaejun Yu, and Y. Kuk, Surface Science **613**, 54 - 57 (2013.Mar). doi: [10.1016/j.susc.2013.03.013](https://doi.org/10.1016/j.susc.2013.03.013)
44. "Crystal-Field Splitting and Correlation Effect on the Electronic Structure of A_2IrO_3 ", H. Gretarsson, J. P. Clancy, X. Liu, J. P. Hill, Emil Bozin, Yogesh Singh, S. Manni, P. Gegenwart, Jungho Kim, A. H. Said, D. Casa, T. Gog, M. H. Upton, Heung-Sik Kim, Jaejun Yu, Vamshi M. Katukuri, L. Hozoi, Jeroen van den Brink, and Young-June Kim, Phys. Rev. Lett. **110**, 076402 (2013.Feb). doi: [10.1103/PhysRevLett.110.076402](https://doi.org/10.1103/PhysRevLett.110.076402)
45. "Physical properties of transparent perovskite oxides $(\text{Ba},\text{La})\text{SnO}_3$ with high electrical mobility at room temperature", Hyung Joon Kim, Useong Kim, Tai Hoon Kim, Jiyeon Kim, Hoon Min Kim, Byung-Gu Jeon, Woong-Jhae Lee, Hyo Sik Mun, Kwang Taek Hong, Jaejun Yu, Kookrin Char, and Kee Hoon Kim, Phys. Rev. B **86**, 165205 (2012.Oct). doi: [10.1103/PhysRevB.86.165205](https://doi.org/10.1103/PhysRevB.86.165205)
46. "Spin and orbital angular momentum structure of $\text{Cu}(111)$ and $\text{Au}(111)$ surface states", Beomyoung Kim, Choong H. Kim, Panjin Kim, Wonsig Jung, Yeongkwan Kim, Yoonyoung Koh, Masashi Arita, Kenya Shimada, Hirofumi Namatame, Masaki Taniguchi, Jaejun Yu, and Changyoung Kim, Phys. Rev. B **85**, 195402 (2012.May). doi: [10.1103/PhysRevB.85.195402](https://doi.org/10.1103/PhysRevB.85.195402)
47. "Effective Control of the Charge and Magnetic States of Transition-Metal Atoms on Single-Layer Boron Nitride", Bing Huang, Hongjun Xiang, Jaejun Yu, and Su-Huai Wei, Phys. Rev. Lett. **108**, 206802 (2012.May). doi: [10.1103/PhysRevLett.108.206802](https://doi.org/10.1103/PhysRevLett.108.206802)
48. "Topological Quantum Phase Transition in 5d Transition Metal Oxide Na_2IrO_3 ", Choong H. Kim, Heung Sik Kim, Hogyun Jeong, Hosub Jin, and Jaejun Yu, Phys. Rev. Lett. **108**, 106401 (2012.Mar). doi: [10.1103/PhysRevLett.108.106401](https://doi.org/10.1103/PhysRevLett.108.106401)
49. "X-ray absorption spectroscopy studies of spin-orbit coupling in 5d transition metal oxides", Deok-Yong Cho, Junghwan Park, Jaejun Yu, and Je-Geun Park, Journal of Physics: Condensed Matter **24**, 055503 (2012.1). doi:
50. "Formation of oxygen vacancies and charge carriers induced in the n-type interface of a LaAlO_3 overlayer on $\text{SrTiO}_3(001)$ ", Yun Li, Sutassana Na Phattalung, Sukit Limpijumnong, Jiyeon Kim, and Jaejun Yu, Phys. Rev. B **84**, 245307 (2011.Dec). doi: [10.1103/PhysRevB.84.245307](https://doi.org/10.1103/PhysRevB.84.245307)
51. "Spin cluster operator theory for the kagome lattice antiferromagnet", Kyusung Hwang, Yong Baek Kim, Jaejun Yu, and Kwon Park, Phys. Rev. B **84**, 205133 (2011.Nov). doi: [10.1103/PhysRevB.84.205133](https://doi.org/10.1103/PhysRevB.84.205133)
52. "Orbital-Angular-Momentum Based Origin of Rashba-Type Surface Band Splitting", Seung Ryong Park, Choong H. Kim, Jaejun Yu, Jung Hoon Han, and Changyoung Kim, Phys. Rev. Lett. **107**, 156803 (2011.Oct). doi: [10.1103/PhysRevLett.107.156803](https://doi.org/10.1103/PhysRevLett.107.156803)
53. "Strain control of magnetism in graphene decorated by transition-metal atoms", Bing Huang, Jaejun Yu, and Su-Huai Wei, Phys. Rev. B **84**, 075415 (2011.Aug). doi: [10.1103/PhysRevB.84.075415](https://doi.org/10.1103/PhysRevB.84.075415)
54. "Defect-related room-temperature ferroelectricity in tensile-strained SrTiO_3 thin films on $\text{GdScO}_3(110)$ substrates", Yong Su Kim, J. S. Choi, J. Kim, S. J. Moon, B. H. Park, J. Yu, J.-H. Kwon, M. Kim, J.-S. Chung, T. W. Noh, and J.-G. Yoon, Applied Physics Letters **97**, 242907 (2010.Dec). doi: [10.1063/1.3525963](https://doi.org/10.1063/1.3525963)

55. "Tunable charge donation and spin polarization of metal adsorbates on graphene using an applied electric field", Jae-Hyeon Parq, Jaejun Yu, Young-Kyun Kwon, and Gunn Kim, Phys. Rev. B **82**, 193406 (2010.Nov). doi: [10.1103/PhysRevB.82.193406](https://doi.org/10.1103/PhysRevB.82.193406)
56. "Electronic structure of double perovskite A_2FeReO_6 ($A = Ba$ and Ca): interplay between spin-orbit interaction, electron correlation, and lattice distortion", B. C. Jeon, Choong H. Kim, S. J. Moon, Woo Seok Choi, Hogyun Jeong, Y. S. Lee, J. Yu, C. J. Won, J. H. Jung, N. Hur, and T. W. Noh, Journal of Physics: Condensed Matter **22**, 345602 (2010.9). doi: [10.1088/0953-8984/22/34/345602](https://doi.org/10.1088/0953-8984/22/34/345602)
57. "Polarization screening and induced carrier density at the interface of $LaAlO_3$ overlayer on $SrTiO_3$ (001)", Yun Li and Jaejun Yu, Journal of Applied Physics **108**, 013701 (2010.7). doi: [10.1063/1.3455877](https://doi.org/10.1063/1.3455877)
58. "Effect of on-site Coulomb interactions on the electronic structure and magnetic property of Gd_2 cluster", Myung Joon Han, Taisuke Ozaki, and Jaejun Yu, Chemical Physics Letters **492**, 89--92 (2010.4). doi: [10.1016/j.cplett.2010.04.018](https://doi.org/10.1016/j.cplett.2010.04.018)
59. "Mapping Atomic Contact between Pentacene and a Au Surface using Scanning Tunneling Spectroscopy", Young Jae Song, Kyuho Lee, Seong Heon Kim, Byoung-Young Choi, Jaejun Yu, and Young Kuk, Nano Letters **10**, 996--999 (2010.02). doi: [10.1021/nl904119y](https://doi.org/10.1021/nl904119y)
60. "First-principles study of ultrathin (2x2) Gd nanowires encapsulated in carbon nanotubes", Jae-Hyeon Parq, Jaejun Yu, and Gunn Kim, The Journal of Chemical Physics **132**, 054701 (2010.02). doi: [10.1063/1.3298693](https://doi.org/10.1063/1.3298693)
61. "Two-Dimensional Confinement of 3d1 Electrons in $LaTiO_3/LaAlO_3$ Multilayers", S. S. A. Seo, M. J. Han, G. W. J. Hassink, W. S. Choi, S. J. Moon, J. S. Kim, T. Susaki, Y. S. Lee, J. Yu, C. Bernhard, H. Y. Hwang, G. Rijnders, D. H. A. Blank, B. Keimer, and T. W. Noh, Phys. Rev. Lett. **104**, 036401 (2010.01). doi: [10.1103/PhysRevLett.104.036401](https://doi.org/10.1103/PhysRevLett.104.036401)
62. "Double polarization hysteresis loop induced by the domain pinning by defect dipoles in $HoMnO_3$ epitaxial thin films", D. Lee, H. S. Kim, S. Y. Jang, K. W. Joh, T. W. Noh, J. Yu, C. E. Lee, and J.-G. Yoon, Phys. Rev. B **81**, 012101 (2010.01). doi: [10.1103/PhysRevB.81.012101](https://doi.org/10.1103/PhysRevB.81.012101)
63. "Structure and magnetism of small Gd and Fe nanoclusters: LDA+U calculations", Gunn Kim, Yongjin Park, Myung Joon Han, Jaejun Yu, Chaejeong Heo, and Young Hee Lee, Solid State Communications **149**, 2058 (2009.12).
64. "Temperature dependence of the electronic structure of the $Jeff = 1/2$ Mott insulator Sr_2IrO_4 studied by optical spectroscopy", S. J. Moon, Hosub Jin, W. S. Choi, J. S. Lee, S. S. A. Seo, J. Yu, G. Cao, T. W. Noh, and Y. S. Lee, Physical Review B **80**, 195110 (2009.11). doi: [10.1103/PhysRevB.80.195110](https://doi.org/10.1103/PhysRevB.80.195110)
65. "Anisotropic exchange interactions of spin-orbit-integrated states in Sr_2IrO_4 ", Hosub Jin, Hogyun Jeong, Taisuke Ozaki and Jaejun Yu, Physical Review B **80**, 075112 (2009.8). doi: [10.1103/PhysRevB.80.075112](https://doi.org/10.1103/PhysRevB.80.075112)
66. "Fundamental thickness limit of itinerant ferromagnetic $SrRuO_3$ thin films", Young Jun Chang, Choong H. Kim, S.-H. Phark, Y. S. Kim, J. Yu, and T. W. Noh, Phys. Rev. Lett. **103**, 057201 (2009.7). doi: [10.1103/PhysRevLett.103.057201](https://doi.org/10.1103/PhysRevLett.103.057201)
67. "Localized electronic states induced by defects and possible origin of ferroelectricity in strontium titanate thin films", Y. S. Kim, J. Kim, S. J. Moon, W. S. Choi, Y. J. Chang, J.-G. Yoon, J. Yu, J.-S. Chung, and T. W. Noh, Applied Physics Letters **94**, 202906 (2009.5). doi: [10.1063/1.3139767](https://doi.org/10.1063/1.3139767)
68. "Competition between structural distortion and magnetic moment formation in fullerene C_{20} ", Myung Joon Han, Gunn Kim, Jae Il Lee, and Jaejun Yu, The Journal of Chemical Physics **130**, 184107 (2009.5). doi: [10.1063/1.3119485](https://doi.org/10.1063/1.3119485)
69. "Possible origins of defect-induced magnetic ordering in carbon-irradiated graphite", Hosik Lee, Yoshiyuki Miyamoto, and Jaejun Yu, Physical Review B (Condensed Matter and Materials Physics) **79**, 121404 (2009.3). doi: [10.1103/PhysRevB.79.121404](https://doi.org/10.1103/PhysRevB.79.121404)

70. "Origin of reduced polarizations in short-period BaTiO₃/SrTiO₃ ferroelectric superlattices", Jun Hee Lee, Jaejun Yu, and U. V. Waghmare, Journal of Applied Physics **105**, 016104 (2009.1). doi: [10.1063/1.3056388](https://doi.org/10.1063/1.3056388)
71. "Dimensionality-Controlled Insulator-Metal Transition and Correlated Metallic State in 5d Transition Metal Oxides Sr_{n+1}Ir_nO_{3n+1} ($n = 1, 2$, and [∞])", S. J. Moon, H. Jin, K. W. Kim, W. S. Choi, Y. S. Lee, J. Yu, G. Cao, A. Sumi, H. Funakubo, C. Bernhard, and T. W. Noh, Physical Review Letters **101**, 226402 (2008.11). doi: [10.1103/PhysRevLett.101.226402](https://doi.org/10.1103/PhysRevLett.101.226402)
72. "Breakdown of half-metallic ferromagnetism in zinc-blende II-V compounds: First-principles calculations", Yun Li and Jaejun Yu, Physical Review B (Condensed Matter and Materials Physics) **78**, 165203 (2008.10). doi: [10.1103/PhysRevB.78.165203](https://doi.org/10.1103/PhysRevB.78.165203)
73. "Novel Jeff = 1/2 Mott State Induced by Relativistic Spin-Orbit Coupling in Sr₂IrO₄", B. J. Kim, Hosub Jin, S. J. Moon, J.-Y. Kim, B.-G. Park, C. S. Leem, Jaejun Yu, T. W. Noh, C. Kim, S.-J. Oh, J.-H. Park, V. Durairaj, G. Cao, and E. Rotenberg, Physical Review Letters **101**, 076402 (2008.8). doi: [10.1103/PhysRevLett.101.076402](https://doi.org/10.1103/PhysRevLett.101.076402)
74. "Electronic Structure and Insulating Nature of the (LaTiO₃)₂/(LaAlO₃)₂ Superlattice", Myung Joon Han and Jaejun Yu, Journal of Korean Physics Society **53**, (2008.08).
75. "First-principles effective Hamiltonian for ferroelectric polarization in BaTiO₃/SrTiO₃ superlattices", Jun Hee Lee, Umesh V. Waghmare, and Jaejun Yu, Journal of Applied Physics **103**, 124106 (2008.6). doi: [10.1063/1.2939588](https://doi.org/10.1063/1.2939588)
76. "Photonic crystal alloys: a new twist in controlling photonic band structure properties", Hee J. Kim, Dong-Uk Kim, Young-Geun Roh, Jaejun Yu, Heonsu Jeon, and Q-Han Park, Opt. Express **16**, 6579--6585 (2008.4). doi: [10.1364/OE.16.006579](https://doi.org/10.1364/OE.16.006579)
77. "Interaction and ordering of vacancy defects in NiO", Sohee Park, Hyo-Shin Ahn, Choong-Ki Lee, Hanchul Kim, Hosub Jin, Hyo-Sug Lee, Sunae Seo, Jaejun Yu, and Seungwu Han, Physical Review B **77**, 134103 (2008.4). doi: [10.1103/PhysRevB.77.134103](https://doi.org/10.1103/PhysRevB.77.134103)
78. "Doped valence-bond solid and superconductivity on the Shastry-Sutherland lattice", Bohm-Jung Yang, Yong Baek Kim, Jaejun Yu, and Kwon Park, Physical Review B (Condensed Matter and Materials Physics) **77**, 104507 (2008.3). doi: [10.1103/PhysRevB.77.104507](https://doi.org/10.1103/PhysRevB.77.104507)
79. "Spin triplet excitations for a valence bond solid on the kagome lattice", Bohm-Jung Yang, Yong Baek Kim, Jaejun Yu, and Kwon Park, Physical Review B (Condensed Matter and Materials Physics) **77**, 224424 (2008.3). doi: [10.1103/PhysRevB.77.224424](https://doi.org/10.1103/PhysRevB.77.224424)
80. "Electronic structures of hexagonal RMnO₃ (R = Gd, Tb, Dy, and Ho) thin films: Optical spectroscopy and first-principles calculations", Woo Seok Choi, Dong Geun Kim, Sung Seok A. Seo, Soon Jae Moon, Daesu Lee, Jung Hyuk Lee, Ho Sik Lee, Deok-Yong Cho, Yun Sang Lee, Pattukkannu Murugavel, Jaejun Yu, and Tae W. Noh, Physical Review B (Condensed Matter and Materials Physics) **77**, 045137 (2008.1). doi: [10.1103/PhysRevB.77.045137](https://doi.org/10.1103/PhysRevB.77.045137)
81. "A Spin-Dependent Local Moment Approach to the Anderson Impurity Model", Choong H. Kim and Jaejun Yu, J. Phys.: Condens. Matter **19**, 456203 (2007.11). doi: [10.1088/0953-8984/19/45/456203](https://doi.org/10.1088/0953-8984/19/45/456203)
82. "Interface electronic structure, two-dimensional metallicity, and possible interface superconductivity in CuCl/Si superlattices", S. H. Rhim, R. Saniz, Jaejun Yu, Lin-Hui Ye, and A. J. Freeman, Physical Review B (Condensed Matter and Materials Physics) **76**, 184505 (2007.11). doi: [10.1103/PhysRevB.76.184505](https://doi.org/10.1103/PhysRevB.76.184505)
83. "Formation of carbon nanotube semiconductor-metal intramolecular junctions by self-assembly of vacancy defects", Gun-Do Lee, Cai-Zhuang Wang, Jaejun Yu, Euijoon Yoon, Nong-Moon Hwang, and Kai-Ming Ho, Physical Review B (Condensed Matter and Materials Physics) **76**, 165413 (2007.10). doi: [10.1103/PhysRevB.76.165413](https://doi.org/10.1103/PhysRevB.76.165413)
84. "Ferroelectricity in Artificial Bicolor Oxide Superlattices", S.S.A. Seo, J.H. Lee, H.N. Lee, M.F. Chisholm, W.S. Choi, D.J. Kim, J.Y. Jo, H. Kim, Jaejun Yu, and T.W. Noh, Advanced Materials **19**, 2460--2464 (2007.9). doi: [10.1002/adma.200601357](https://doi.org/10.1002/adma.200601357)

85. "Enhanced Charge Gap in the Bilayer Manganite $La_{2-x}Sr_{1+2x}Mn_2O_7$ near $x = 0.4$ ", Myung Whun Kim, H. J. Lee, B. J. Yang, K. H. Kim, Y. Moritomo, Jaejun Yu, and T. W. Noh, Physical Review Letters **98**, 187201 (2007.May). doi: [10.1103/PhysRevLett.98.187201](https://doi.org/10.1103/PhysRevLett.98.187201)
86. "Pseudogap Dependence of the Optical Conductivity Spectra of $Ca_3Ru_2O_7$: A Possible Contribution of the Orbital Flip Excitation", J. S. Lee, S. J. Moon, B. J. Yang, Jaejun Yu, U. Schade, Y. Yoshida, S.-I. Ikeda, and T. W. Noh, Physical Review Letters **98**, 97403 (2007.3). doi: <http://link.aps.org/abstract/PRL/v98/e097403>
87. "Magnetic ordering and exchange interactions in multiferroic $GaFeO_3$ ", Myung Joon Han, Taisuke Ozaki, and Jaejun Yu, Physical Review B **75**, 060404(R) (2007.2). doi: [10.1103/PhysRevB.75.060404](https://doi.org/10.1103/PhysRevB.75.060404)
88. "Comparison of localized basis and plane-wave basis for density-functional calculations of organic molecules on metals", Kyuho Lee, Jaejun Yu, and Yoshitada Morikawa, Physical Review B (Condensed Matter and Materials Physics) **75**, 045402 (2007.1). doi: <http://link.aps.org/abstract/PRB/v75/e045402>
89. "Synthesis, Characterization, and Self-Assembly of Pencil-Shaped CoO Nanorods", Kwangjin An, Nohyun Lee, Jongnam Park, Sung Chul Kim, Yosun Hwang, Je-Geun Park, Jae-Young Kim, Jae-Hoon Park, Myung Joon Han, Jaejun Yu and Taeghwan Hyeon, Journal of the American Chemical Society **128**, 9753-9760 (2006). doi: [10.1021/ja0608702](https://doi.org/10.1021/ja0608702)
90. "O(N) LDA+U electronic structure calculation method based on the non-orthogonal pseudo-atomic orbital basis", Myung Joon Han, Taisuke Ozaki and Jaejun Yu, Phys. Rev. B **73**, 45110 (2006).
91. "Electronic Structure and Magnetic Properties of Wurtzite CoO ", Myung Joon Han and Jaejun Yu, Journal of the Korean Physical Society **48**, 1496-1500 (2006).
92. "Missing xy-Band Fermi Surface in 4d Transition-Metal Oxide Sr_2RhO_4 : Effect of the Octahedra Rotation on the Electronic Structure", B. J. Kim, Jaejun Yu, H. Koh, I. Nagai, S. I. Ikeda, S.-J. Oh and C. Kim, Physical Review Letters **97**, 106401 (2006).
93. "Effect of Orbital Rotation and Mixing on the Optical Properties of Orthorhombic $RMnO_3$ ($R = La, Pr, Nd, Gd, and Tb$)", M. W. Kim, S. J. Moon, J. H. Jung, Jaejun Yu, Sachin Parashar, P. Murugavel, J. H. Lee and T. W. Noh, Physical Review Letters **96**, 247205 (2006).
94. "Electronic structure and magnetic properties of small manganese", Myung Joon Han, Taisuke Ozaki and Jaejun Yu, J. Chem. Phys. **123**, 34306 (2005).
95. "Magnetic ordering at the edges of graphitic fragments: Magnetic tail interactions between the edge-localized states", Hosik Lee, Young-Woo Son, Noejung Park, Seungwu Han and Jaejun Yu, Phys. Rev. B **72**, 174431 (2005).
96. "Ab initio study of pentacene on Au(001) surface", Kyuho Lee and Jaejun Yu, Surface Science **589**, 8 - 18 (2005).
97. "Band gap sensitivity of bromine adsorption at carbon nanotubes", Noejung Park, Yoshiyuki Miyamoto, Kyuho Lee, Wooni Ih Choi, Jisoon Ihm, Jaejun Yu and Seungwu Han, Chemical Physics Letters **403**, 135 - 139 (2005).
98. "Electronic structure, magnetic interactions, and the role of ligands in M_{nn} ($n = 4, 12$) single-molecule magnets", Myung Joon Han, Taisuke Ozaki and Jaejun Yu, Phys. Rev. B **70**, 184421 (2004).
99. "Interplay between spin and orbital configurations in a pyrochlore molybdate studied by optical spectroscopy", M.W. Kim, Y.S. Lee, T.W. Noh, Jaejun Yu and Y. Moritomo, Ann. Phys. (Leipzig) **13**, 76 - 77 (2004).
100. "Optical spectroscopic detection of spin exchange interaction in pyrochlore molybdates", M. W. Kim, Y. S. Lee, T. W. Noh, Jaejun Yu and Y. Moritomo, Phys. Rev. Lett. **92**, 27202 (2004).
101. "Ferromagnetism at the edges of the stacked graphitic fragments: an ab initio study", Hosik Lee, Noejung Park, Young-Woo Son, Seungwu Han and Jaejun Yu, Chem. Phys. Lett. **398**, 207 - 211 (2004).

102. "Bond-length dependence of charge-transfer excitations and stretch phonon modes in perovskite ruthenates: Evidence of strong p-d hybridization effects", J.S. Lee, Y.S. Lee, T.W. Noh, S. Nakatsuji, H. Fukazawa, R.S. Perry, Y. Maeno, Y. Yoshida, S.I. Ikeda, Jaejun Yu and C.B. Eom, Phys. Rev. B **70**, 85103 (2004).
103. "Heat-Induced Transformation of Nanodiamond into a Tube-Shaped Fullerene: A Molecular Dynamics Simulation", G.-D. Lee, C. Z. Wang, Jaejun Yu, E. Yoon and K. M. Ho, Phys. Rev. Lett. **91**, 265701 (2003).
104. "Dynamic Jahn-Teller Effect and Superconductivity in MgB₂", Jaejun Yu, Young Woo Son and Jisoon Ihm, Physica C **388--389**, 135 - 136 (2003).
105. "Spin-Orbital Pattern Dependent Polaron Absorption in Manganites", M. W. Kim, J. H. Jung, K. H. Kim, H. J. Lee, Jaejun Yu, T. W. Noh and Y. Moritomo, Phys. Rev. Lett. **89**, 16403 (2002).
106. "Ultraviolet photoelectron spectroscopy study of colossal magnetoresistive La_{0.7-x}P_xCa_{0.3}MnO₃", C.-W. Lee, Y.D. Zhao, H. Koh, H.-J. Noh, J. Park, H.-D. Kim, Jaejun Yu, S.-J. Oh and M. Han, Solid State Commun. **123**, 11 - 15 (2002).
107. "Catalytic Decomposition Of Acetylene On Fe(001): A First-Principles Study", G.-D. Lee, S. Han, Jaejun Yu and J. Ihm, Phys. Rev. B **66**, 081403(R) (2002).
108. "Electron and Orbital Correlations in Ca_{2-x}S_xRuO₄ Probed by Optical Spectroscopy", J. S. Lee, Y. S. Lee, T. W. Noh, S.-J. Oh, Jaejun Yu, S. Nakatsuji, H. Fukazawa and Y. Maeno, Phys. Rev. Lett. **89**, 257402 (2002).
109. "Non-Fermi liquid behavior and scaling of the low-frequency suppression in the optical conductivity spectra of CaRuO₃", Y.S. Lee, Jaejun Yu, J.S. Lee, T.W. Noh, T.-H. Gimm, Han-Yong Choi and C.B. Eom, Phys. Rev. B. **66**, 041104(R) (2002).
110. "Energetics of large carbon clusters: Crossover from fullerenes to nanotubes", N. Park, K. Lee, S. Han, Jaejun Yu and Jisoon Ihm, Phys. Rev. B **65**, 121405 (2002).
111. "Temperature-dependent self-doping effects on the metal-insulator transition of Tl₂Ru₂O₇", J.S. Lee, Y.S. Lee, K.W. Kim, T.W. Noh, Jaejun Yu, T. Takeda and R. Kanno, Phys. Rev. B **64**, 165108 (2001).
112. "Optical investigation of A₂Ru₂O₇ (A=Y, Tl, and Bi): temperature dependent self-doping effects", J.S. Lee, Y.S. Lee, K.W. Kim, T.W. Noh, Jaejun Yu, Y. Takeda and R. Kanno, Physica C **364--365**, 632 - 635 (2001).
113. "Pseudogap formation in four-layer BaRuO₃ and its electrodynamic response changes", Y.S. Lee, J.S. Lee, K.W. Kim, T.W. Noh, Jaejun Yu, Yunkyu Bang, M.K. Lee and C.B. Eom, Phys. Rev. B **64**, 165109 (2001).
114. "Pseudogap formation in 4d transition metal oxide BaRuO₃", Y.S. Lee, J.S. Lee, K.W. Kim, T.W. Noh, Jaejun Yu, E.J. Choi, G. Cao and J.E. Crow, Europhysics Letters **55**, 280 - 286 (2001).
115. "BaRuO₃: a new type of pseudogap systems", T.W. Noh, Y.S. Lee, J.S. Lee, K.W. Kim, Jaejun Yu, G. Cao, J.E. Crow, M.K. Lee and C.B. Eom, Physica C **364--365**, 480 - 483 (2001).
116. "Optical properties of BaRuO₃: observation of pseudogap formation", T.W. Noh, Y.S. Lee, J.S. Lee, K.W. Kim, Jaejun Yu, G. Cao, J.E. Crow, M.K. Lee and C.B. Eom, Current Applied Physics **1**, 163 - 167 (2001).
117. "Optical investigations of the charge gap in orbital-ordered La_{1/2}Sr_{3/2}MnO₄", J.H. Jung, J.S. Ahn, Jaejun Yu, T.W. Noh, J. Lee, Y. Moritomo, I. Solovyev and K. Terakura, Physical Review B- Condensed Matter **61**, 6902 - 6906 (2000).
118. "Dimensional crossover driven by magnetic ordering in optical conductivity of Pr_{1/2}Sr_{1/2}MnO₃", J. H. Jung, H. J. Lee, Jaejun Yu, T. W. Noh, E. J. Choi and Y. Moritomo, Physical Review B- Condensed Matter **61**, 14656 - 14659 (2000).
119. "Optical Properties of Perovskite Manganites", T.W. Noh, J.H. Jung, H.J. Lee, K.H. Kim, Jaejun Yu, E.J. Choi and Y. Moritomo, Journal of Korean Physics Society **36**, 392 - 397 (2000).

120. "Anomalous spin susceptibility and magnetic polaron formation in the double-exchange systems", Hongsuk Yi, N. H. Hur and Jaejun Yu, Physical Review B-Condensed Matter **61**, 9501 - 9505 (2000).
121. "Long-range hopping correlation and colossal magnetoresistance in doped manganites", Hongsuk Yi, N H Hur and Jaejun Yu, Journal of Physics-Condensed Matter **12**, 5453 - 5462 (2000).
122. "Magnetic Phase Diagram of the Anisotropic Double-Exchange Model: A Monte Carlo Study", Hongsuk Yi, Jaejun Yu and N. H. Hur, Journal of the Korean Physical Society **37**, 114 - 118 (2000).
123. "Suppression of ferromagnetic ordering in doped manganites: Effects of the superexchange interaction", Hongsuk Yi, Jaejun Yu and Sung-Ik Lee, Physical Review B-Condensed Matter **61**, 428 - 431 (2000).
124. "Observation of low field magnetoresistance in the layered manganite $Sr_{1.6}Sm_{1.4}Mn_2O_7$ ", N.H. Hur, E.O. Chi, Y.U. Kwon, Jaejun Yu, J.-T. Kim, Y.K. Park and J.C. Park, Solid State Communications **112**, 61 - 65 (1999).
125. "Orbital and charge orderings and magnetism in perovskite-type transition-metal oxides", K. Terakura, J. Lee, Jaejun Yu, I.V. Solovyev and H. Sawada, Materials Science and Engineering B-Solid State Materials for Advanced Tech **63**, 11 - 16 (1999).
126. "Coexistence of antiferromagnetic and ferromagnetic phase for ferromagnetic Kondo lattice model", H. Yi, Jaejun Yu and S.-I. Lee, European Physical Journal B **7**, 509 - 512 (1999).
127. "Midgap states of $La_{1-x}Ca_xMnO_3$: Doping-dependent optical-conductivity studies", J.H. Jung, K.H. Kim, T.W. Noh, E.J. Choi and Jaejun Yu, Physical Review B-Condensed Matter **57**, R11043 - 11046 (1998).
128. "Scaling Behavior of Spectral Weight Changes in Perovskite Manganites $La_{0.7-y}PryCa_{0.3}MnO_3$ ", K.H. Kim, J.H. Jung, D.J. Eom, T.W. Noh, Jaejun Yu and E.J. Choi, Physical Review Letters **81**, 4983 - 4986 (1998).
129. "Density Functional Study of Lattice Distortion and Orbital Ordering in $La_{1-x}Ca_{1+x}MnO_4$ ", Jinhyoung Lee, Jaejun Yu and K. Terakura, J. Korean Phys. Soc. **33**, S55 - 58 (1998).
130. "Double-exchange model with background superexchange interactions: Phase diagrams of $La_{1-x}Ca_xMnO_3$ manganites", Hongsuk Yi and Jaejun Yu, Physical Review B-Condensed Matter **58**, 11123 - 11126 (1998).
131. "Determination of electronic band structures of $CaMnO_3$ and $LaMnO_3$ using optical-conductivity analyses", J.H. Jung, K.H. Kim, D.J. Eom, T.W. Noh, E.J. Choi, Jaejun Yu, Y.S. Kwon and Y. Chung, Phys. Rev. B **55**, 15489 (1997).
132. "Induced vortex dynamics in parallel Josephson junction arrays", Jinhyoung Lee, Jaejun Yu and Gwangseo Park, Phys. Rev. B **55**, 1231 (1997).
133. "Grand Canonical Quantum Monte Carlo Methods: An Application to the 1D Hubbard Model", Hongsuk Yi and Jaejun Yu, J. Kor. Phys. Soc. **31**, 315 (1997).
134. "First principles total energy study of ferroelectric transitions in $LiNbO_3$ ", Jaejun Yu and Key-Taeck Park, Physica B **237--238**, 341 (1997).
135. "Dynamical properties of HTSC granular bridge junctions: inhomogeneous Josephson junction array model", Jihyoung Lee, Sangmin Lee, Jaejun Yu and Gwangseo Park, Phys. Rev. B **53**, 3578 (1996).
136. "Pressure induced phonon softening and electronic topological transition in $HgBa_2CuO_4$ ", D.L. Novikov, M.I. Katsnelson, A.V. Postnikov, Jaejun Yu and A.J. Freeman, Phys. Rev. B **54**, 1313 (1996).
137. "FLAPW Total Energy Study of Electronic Structure and Ferroelectric Distortions of $LiNbO_3$ ", Jaejun Yu and Key-Taeck Park, J. Kor. Phys. Soc. **29**, S603 (1996).

138. "Order parameter relaxation effects on the I-V characteristics of high-T_c Josephson junctions", Gwang-Hee Kim and Jaejun Yu, *Physica C* **253**, 139 - 146 (1995).
139. "Current-Voltage Characteristics and Josephson AC Effects of Granular HTSC Y₁Ba₂Cu₃O_y Bridges", S. Lee, H. Kim, D. Song, Jaejun Yu and G. Park, *Solid State Communications* **94**, 45 - 48 (1995).
140. "A Raman study on the effects of pressure in HgBa₂Ca_{n-1}Cu_nO_{2n+2+d} superconductors and related compounds", I.-S. Yang, H.-G. Lee, H.-S. Shin, S.-J. Jeon, H.-S. Ahn, Jaejun Yu, N.H. Hur and S.-I. Lee, *J. Korean Phys. Soc.* **28**, S224 (1995).
141. "Raman modes of the apical oxygen in mercury-based superconductors", I.S. Yang, H.-G. Lee, Jaejun Yu and N.H. Hur, *Phys. Rev. B* **52**, 15078 (1995).
142. "A micro-Raman study on the role of pressure in mercury-based superconductors", I.-S. Yang, H.-S. Shin, H.-G. Lee, S.-J. Jeon, H.S. Ahn, Jaejun Yu, S. Lee and S.-I. Lee, *Phys. Rev. B* **51**, 644 (1995).
143. "A micro-Raman study on the role of pressure in mercury-based superconductors", I.-S. Yang, H.-S. Shin, H.-G. Lee, S.-J. Jeon, H.S. Ahn, Jaejun Yu, S. Lee and S.-I. Lee, *Phys. Rev. B* **51**, 644 (1995).
144. "Total energy frozen phonon calculations of HgBa₂CuO₄", Jaejun Yu, *J. Kor. Phys. Soc.* **28**, S292 (1995).
145. "Orientations of Oxygen Hole States and Ionicity of Bismuth Atoms in Bi₂Sr₂CaCu₂O₈", M. Faiz, G. Jennings, J.C. Campuzano, E.E. Alp, J.M. Yao, D.K. Saldin and Jaejun Yu, *Phys. Rev. B* **50**, 6370 (1994).
146. "Raman mode assignments of HgBa₂CuO₄ Crystallites", H.-G. Lee, H.-S. Shin, I.-S. Yang, Jaejun Yu and N.H. Hur, *Physica C* **233**, 35-39 (1994).
147. "Electronic Band Structure of High T_c Cu-Oxide Superconductors: Comparison of Predictions with Experiments", Jaejun Yu and A. J. Freeman, *J. Electron Spectroscopy and Related Phenomena* **66**, 281 (1994).
148. "Electronic Structure and Properties of Vacancy-Ordered YBa₂Cu₃O_{6.5}: Chain vs Plane Fermi Surfaces in YBa₂Cu₃O_{7-d}", Jaejun Yu, S. Massidda, A. J. Freeman and R. Podloucky, *Physica C* **214**, 335 - 344 (1993).
149. "Two-Photon Momentum Density in La_{2-x}S_xCuO₄ and Nd_{2-x}C_xCuO₄", P. Blandin, S. Massidda, B. Barbiellini, T. Jarlborg, P. Lerch, A.A. Manuel, L. Hoffmann, M. Gauthier, W. Sadowski, E. Walker, M. Peter, Jaejun Yu and A.J. Freeman, *Phys. Rev. B* **46**, 390 (1992).
150. "Hole states in CuO₂ planes and Cu-O chains of YBa₂Cu₃O₇ and YBa₂Cu₄O₈ probed by soft-X-ray absorption spectroscopy", A. Krol, Z.H. Ming, Y.H. Kao, N. N G. Roth, J. Fink, G.C. Smith, Key Taeck Park, Jaejun Yu, A.J. Freeman, A. Erband, G. MVogt, J. Karpinski, E. Kaldis and K. Schonmann, *Phys. Rev. B* **45**, 2581 (1992).
151. "Theoretical Two-Particle Momentum Density in YBa₂Cu₃O_{7-d}", S. Massidda, Jaejun Yu, A.J. Freeman, L. Hoffmann, P. Genoud and A.A. Manuel, *J. Phys. Chem. Solids* **52**, 1503 (1991).
152. "Normal State Transport Properties of the YBa₂Cu₄O₈ and YBa₂Cu₃O₇ Superconductors: Predictions and Comparison with Experiments", S. Massidda, Jaejun Yu, Key Taeck Park and A.J. Freeman, *Physica C* **176**, 159 (1991).
153. "Coulomb Correlated Band Structure and Fermi Surfaces of High T_c Superconductors", Jaejun Yu and A.J. Freeman, *J. Phys. Chem. Solids* **52**, 1351 (1991).
154. "Coulomb Correlated Electronic Band Structure of Cuprate Superconductors", Jaejun Yu and A.J. Freeman, *Physica C* **173**, 274 (1991).
155. "Origin of Electric Field Gradients in High Temperature Superconductors: YBa₂Cu₃O₇", Jaejun Yu, A.J. Freeman, R. Podloucky, P. Herzig and P. Weinberger, *Phys. Rev. B* **43**, 532 (1991).
156. "Electronic Structure and Properties of YBa₂Cu₄O₈", Jaejun Yu, Key Taeck Park and A.J. Freeman, *Physica C* **172**, 467 (1991).
157. "Transport Properties of High-T_c Superconductors", N. Hamada, S. Massidda, Jaejun Yu and A.J. Freeman, *Phys. Rev. B* **42**, 6238 (1990).

- 158."Calculated Photoemission, Inverse Photoemission, and X-ray Emission Spectra of High T_c Superconductors: $Tl_2Ba_2CaCu_2O_8$ and $Tl_2Ba_2Ca_2Cu_3O_{10}$ ", P. Marksteiner, Jaejun Yu, S. Massidda, A.J. Freeman, J. Redinger and P. Weinberger, Phys. Rev. B **39**, 2894 (1989).
- 159."Electronic Structure of Nd-Ce-Cu-O, A Fermi Liquid Superconductor", S. Massidda, N. Hamada, Jaejun Yu and A.J. Freeman, Physica C **157**, 571 (1989).
- 160."Electronic Structure and High T_c Superconductivity in Transition Metal Oxides", A.J. Freeman and Jaejun Yu, Physica B **150**, 50 (1988).
- 161."Energy Band Structure of the High T_c Superconductors", A.J. Freeman and Jaejun Yu, Helvetica Physica Acta **61**, 401 (1988).
- 162."Electronic Structure, Charge Transfer Excitations, and High Temperature Superconducting Oxides", A.J. Freeman, Jaejun Yu, S. Massidda, C.L. Fu and J.H. Xu, J. Appl. Phys. **63**, 4220 (1988).
- 163."Electronic Structure and Properties of $Bi_2Sr_2CaCu_2O_8$, the Third High T_c Superconductor", S. Massidda, Jaejun Yu and A.J. Freeman, Physica C **152**, 251 (1988).
- 164."Electronic Structure and Properties of Superconducting $LiTi_2O_4$ ", S. Massidda, Jaejun Yu and A.J. Freeman, Phys. Rev. B **38**, 11352 (1988).
- 165."Calculated Photoemission and X-ray Emission Spectra of $Bi_2Sr_2CaCu_2O_8$ ", with P. Marksteiner, S. Massidda, Jaejun Yu, A.J. Freeman and J. Redinger, Phys. Rev. B **38**, 5098 (1988).
- 166."Electronic Structure and Properties of High T_c Superconductor $Tl_2Ba_2CaCu_2O_8$ and $Tl_2Ba_2Ca_2Cu_3O_{10}$ ", Jaejun Yu, S. Massidda and A.J. Freeman, Physica C **152**, 273 (1988).
- 167."Electronic Structure and Properties of Quasi-2D Layered Superconducting Perovskite: $La_{2-x}MxCuO_4$ ($M = Sr, Ba, \dots$)", A.J. Freeman, Jaejun Yu and C.L. Fu, Phys. Rev. B **36**, 7111 (1987).
- 168."All-electron Local Density Theory of Electronic Structure and Superconductivity in $YBa_2Cu_3O_7$ and $YBa_2Cu_3O_6$ ", A.J. Freeman, Jaejun Yu, S. Massidda and D.D. Koelling, Jap. J. Appl. Phys. **26**, 1153 (1987).
- 169."Electronic Structure, Charge Transfer Excitations and High Temperature Superconductivity", A.J. Freeman, Jaejun Yu, S. Massidda and D.D. Koelling, Physica B **148**, 212 (1987).
- 170."Electronic Structure and Properties of $YBa_2Cu_3O_{7-d}$, a Low Dimensional, Low Density of States Superconductor", S. Massidda, Jaejun Yu, A.J. Freeman and D.D. Koelling, Phys. Lett. A **122**, 198 (1987).
- 171."Local Density Theory of X-ray and Photoemission From $YBa_2Cu_3O_{7-d}$, The High T_c Superconductor", J. Redinger, A.J. Freeman, Jaejun Yu and S. Massidda, Phys. Lett. A **124**, 469 (1987).
- 172."Calculated Local Density X-ray and Photoemission Spectra for Superconducting $La_{2-x}MxCuO_4$: Localization of Cu-3d", J. Redinger, Jaejun Yu, A.J. Freeman and P. Weinberger, Phys. Lett. A **124**, 463 (1987).
- 173."Dominant Role of the 2D van Hove Singularity on the Fermi Surface and Generalized Susceptibility of the Quasi-2D Superconductor $La_{2-x}MxCuO_4$ ($M = Sr, Ba, \dots$)", J.-H. Xu, T.J. Watson-Yang, Jaejun Yu and A.J. Freeman, Phys. Lett. A **120**, 489 (1987).
- 174."Bonds, Bands, Charge Transfer Excitations and Superconductivity: $YBa_2Cu_3O_{7-d}$ vs. $YBa_2Cu_3O_6$ ", Jaejun Yu, A.J. Freeman and S. Massidda, Novel Superconductivity , 357 (1987).
- 175."Electronically Driven Instabilities and Superconductivity in the Layered $La_{2-x}MxCuO_4$ Perovskites", Jaejun Yu, A.J. Freeman and J.-H. Xu, Phys. Rev. Lett. **58**, 1035 (1987).
- 176."Bonds, Bands, Charge Transfer Excitations and Superconductivity of $YBa_2Cu_3O_{7-d}$ ", Jaejun Yu, S. Massidda, A.J. Freeman and D.D. Koelling, Phys. Lett. A **122**, 203 (1987).