

Manish Jain

Curriculum Vitae

Contact Information

Department of Physics
Indian Institute of Science
Bangalore 560 012 India

Phone: 91-80-2293 2858

Email: mjain@iisc.ac.in

Website: <http://www.physics.iisc.ac.in/~mjain>

Education

Ph.D., Materials Science and Engineering, 6/2002

University of Minnesota, Minneapolis, MN, USA

Thesis: Ab initio simulations for semiconductor liquids

Advisers: Prof. J. R. Chelikowsky and Prof. J. J. Derby

B.Tech., Materials and Metallurgical Engineering, 5/1997

Indian Institute of Technology, Kanpur, India

Thesis: Study of ternary diffusion couples of Ni Al Si

Adviser: Prof. S. P. Gupta

Minor: Solid State and Statistical Physics

Research Experience

12/2018–present Associate Professor
Department of Physics,
Indian Institute of Science
Bangalore 560 012 India

12/2012–12/2018 Assistant Professor
Department of Physics,
Indian Institute of Science
Bangalore 560 012 India

1/2012–11/2012 Postdoctoral Researcher
Institute for Computational Engineering and Science
University of Texas at Austin, USA.
(Adviser : Prof. J. R. Chelikowsky)

Visiting Scholar
Lawrence Berkeley National Laboratory and
Department of Physics, University of California, Berkeley, USA
(Adviser : Prof. S. G. Louie)

- 9/2010–1/2012 Postdoctoral Fellow
Lawrence Berkeley National Laboratory and
Department of Physics, University of California, Berkeley, USA
(Adviser : Prof. S. G. Louie)
- 6/2008–9/2010 Postdoctoral Researcher
Institute for Computational Engineering and Science
University of Texas at Austin, USA.
(Adviser : Prof. J. R. Chelikowsky)
- Visiting Scholar
Lawrence Berkeley National Laboratory and
Department of Physics, University of California, Berkeley, USA
(Adviser : Prof. S. G. Louie)
- 7/2002–5/2008 Senior Research Engineer
Corporate Research Materials Laboratory
3M Company, St. Paul, USA

Professional Activities

Co-organizer and co-convener of conference: “Novel Oxide Materials and Low Dimensional Systems”, The 5th Indian Association for the Cultivation of Science–Asia-Pacific Center for Theoretical Physics international conference in Bangalore, India, December 9–11, 2013.

Co-organizer of school: “Strongly Correlated Systems: From Models to Materials”, International Centre for Theoretical Sciences school in Bangalore, India, January 6–17, 2014.

Co-organizer of conference: “Current Trends in Condensed Matter Physics”, in Bhubaneswar, India, February 19–22, 2015.

Co-organizer of conference: “2nd Annual Conference on Quantum Condensed Matter”, in Bangalore, India, July 8–10, 2019.

Teaching Experience

‘Condensed Matter Physics - I’ – Spring 2014, Spring 2015 and Spring 2016.

‘Computational Physics’ – Spring 2017, Spring 2018, Spring 2019 and jointly in Spring 2020.

‘Quantum Mechanics - I’ – Fall 2019 and Fall 2020.

Graduate/undergraduate Students (current)

Indrajit Maity (PhD student joined August 2015)

Sudipta Kundu (Int PhD student joined August 2015)

Anjali Nair Lalithambika (PhD student joined August 2014 co-advised with Prof. S. Raghavan)

Vivek Singh (PhD student joined August 2016 co-advised with Prof. S. Avasthi)

Sanat K. Gogoi (PhD student joined August 2017)
Shinjan Mandal (PhD student joined August 2018)
Ishita Suhas Shitut (Int PhD student joined August 2018)
Namana Venkatareddy (Int PhD student joined August 2019)
Robin Bajaj (Int PhD student joined August 2020)
S. ShriHari (BS student joined August 2020)

Graduate/undergraduate Students and Research Assistants supervised

Dr. Mit H. Naik (PhD 2014–19)
Dr. Tathagata Biswas (PhD 2013–18)
Dr. Rabeet Singh (Research Assistant 2020)
Vaibhav Sahu (BS 2019–20)
Gourab Panigrahi (MS 2018–19)
Ruman Moulik (BS/MS 2018–20)
Utkarsh Pratiush (BS 2018–19 co-advised with Prof. R. Ranjan)
Mandadi Varuneshwar Reddy (MS 2018–19 co-advised with Prof. H. R. Krishnamurthy)
Gautam Aditya Kavuri (BS 2017–18)
Sudheer Anand Sreedhar (MS 2017–18)
Varshitha Kikkeri Shivalingegowda (BS/MS 2015–17)
Tamoghna Barik (BS 2015–16)
M. Poshit Nag (Research Assistant 2013–15)

Publications

Journal Papers

- [84] Abhishek Aggarwal, Anil Kumar Sahoo, Saientan Bag, Veerabhadrarao Kaliginedi, Manish Jain, and Prabal K. Maiti, *Fine-tuning the DNA conductance by intercalation of drug molecules*, Physical Review E **103**, 032411 (2021).
- [83] Sudipta Kundu, Satadeep Bhattacharjee, Seung-Cheol Lee, and Manish Jain, *Population analysis with Wannier orbitals*, The Journal of Chemical Physics **154**, 104111 (2021).
- [82] Indrajit Maity, Prabal K. Maiti, H. R. Krishnamurthy, and Manish Jain, *Reconstruction of moiré lattices in twisted transition metal dichalcogenide bilayers*, Physical Review B **103**, L121102 (2021).

- [81] Shashank Kumar Ojha, Sanat Kumar Gogoi, Prithwjit Mandal, S. D. Kaushik, J. W. Freeland, M. Jain, and S. Middey, *Oxygen vacancy induced electronic structure modification of $KTaO_3$* , Physical Review B **103**, 085120 (2021).
- [80] Phanibhusan S. Mahapatra, Bhaskar Ghawri, Manjari Garg, Shinjan Mandal, K. Watanabe, T. Taniguchi, Manish Jain, Subroto Mukerjee, and Arindam Ghosh, *Misorientation-Controlled Cross-Plane Thermoelectricity in Twisted Bilayer Graphene*, Physical Review Letters **125**, 226802 (2020).
- [79] Sanjay Nayak, Mit H. Naik, Manish Jain, Umesh V. Waghmare, and Sonnada M. Shivaprasad, *First-principles theoretical analysis and electron energy loss spectroscopy of vacancy defects in bulk and nonpolar $(10\bar{1}0)$ surface of GaN* , Journal of Vacuum Science & Technology A **38**, 063205 (2020).
- [78] Abhishek Aggarwal, Saientan Bag, Ravindra Venkatramani, Manish Jain, and Prabal K. Maiti, *Multiscale modelling reveals higher charge transport efficiencies of DNA relative to RNA independent of mechanism*, Nanoscale **12**, 18750 (2020).
- [77] Mit H. Naik, Sudipta Kundu, Indrajit Maity, and Manish Jain, *Origin and evolution of ultraflat bands in twisted bilayer transition metal dichalcogenides: Realization of triangular quantum dots*, Physical Review B **102**, 075413 (2020).
- [76] Saientan Bag, Tathagata Biswas, Manish Jain, and Prabal K. Maiti, *Anisotropic Charge Transport in Nanoscale DNA Wire*, The Journal of Physical Chemistry C **124**, 16763 (2020).
- [75] Sudipta Kundu, Mit H. Naik, and Manish Jain, *Native point defects in mono and bilayer phosphorene*, Physical Review Materials **4**, 054004 (2020).
- [74] Suman Sarkar, Indrajit Maity, H. L. Pradeepa, Goutham Nayak, Laetitia Marty, Julien Renard, Johann Coraux, Nedjma Bendiab, Vincent Bouchiat, Sarthak Das, et al., *Anharmonicity in Raman-active phonon modes in atomically thin MoS_2* , Physical Review B **101**, 205302 (2020).
- [73] Rahul Debnath, Indrajit Maity, Rabindra Biswas, Varun Raghunathan, Manish Jain, and Arindam Ghosh, *Evolution of high-frequency Raman modes and their doping dependence in twisted bilayer MoS_2* , Nanoscale **12**, 17272 (2020).
- [72] Shashank Kumar Ojha, Sanat Kumar Gogoi, Manju Mishra Patidar, Ranjan Kumar Patel, Prithwjit Mandal, Siddharth Kumar, Radhakrishnan Venkatesh, Vedachalaiyer Ganesan, Manish Jain, and Srimanta Middey, *Oxygen Vacancy-Induced Topological Hall Effect in a Nonmagnetic Band Insulator*, Advanced Quantum Technologies **3**, 2000021 (2020).
- [71] Indrajit Maity, Mit H. Naik, Prabal K. Maiti, H. R. Krishnamurthy, and Manish Jain, *Phonons in twisted transition-metal dichalcogenide bilayers: Ultrasoft phasons and a transition from a superlubric to a pinned phase*, Physical Review Research **2**, 013335 (2020).

- [70] Tanweer Ahmed, Mit H Naik, Simran Kumari, Smriti P Suman, Rahul Debnath, Sudipta Dutta, Umesh V Waghmare, Manish Jain, and Arindam Ghosh, *Thermodynamically stable octahedral MoS₂ in van der Waals hetero-bilayers*, 2D Materials **6**, 041002 (2019).
- [69] Anomitra Sil, Devendra Singh Negi, Mit H. Naik, Manish Jain, Ranjan Datta, Rajeev Ranjan, and P. S. Anil Kumar, *Large intrinsic magnetization in the epitaxial BiFeO₃/NdGaO₃ system*, Europhysics Letters **126**, 57003 (2019).
- [68] Tathagata Biswas and Manish Jain, *Electronic structure and optical properties of F-centers in α -alumina*, Physical Review B **99**, 144102 (2019a).
- [67] Tathagata Biswas and Manish Jain, *Polarization discontinuity driven two dimensional electron gas at A₂Mo₃O₈/B₂Mo₃O₈ (A, B: Zn, Mg, Cd) interfaces*, Journal of Applied Physics **125**, 145303 (2019b).
- [66] Mit H. Naik, Indrajit Maity, Prabal K. Maiti, and Manish Jain, *Kolmogorov-Crespi Potential for Multilayer Transition Metal Dichalcogenides: Capturing Structural Transformations in Moiré Superlattices*, The Journal of Physical Chemistry C **123**, 9770 (2019).
- [65] Pramod Ravindra, Madhusmita Baral, Tathagata Biswas, Mangala Nand, S. N. Jha, Eashwer Athresh, Rajeev Ranjan, Manish Jain, Tapas Ganguli, and Sushobhan Avasthi, *Electrical and optical properties of low-bandgap oxide Zn₂Mo₃O₈ for optoelectronic applications*, Thin Solid Films **677**, 95 (2019).
- [64] Krishna Balasubramanian, Tathagatha Biswas, Priyadarshini Ghosh, Swathi Suran, Rohan Mishra, Ritesh Sachan, Manoj Varma, Manish Jain, Rudra Pratap, and Srinivasan Raghavan, *Reversible Engineering of Grain Boundary Defects in Graphene*, Nature Communications **10**, 1090 (2019).
- [63] K C Krishnapriya, Palas Roy, Boregowda Puttaraju, Ulrike Salzner, Andrew J Musser, Manish Jain, Jyotishman Dasgupta, and Satish Patil, *Spin Density Encodes Intramolecular Singlet Exciton Fission in Pentacene Dimers*, Nature Communications **10**, 33 (2019).
- [62] Mit H. Naik and Manish Jain, *Ultraflatbands and Shear Solitons in Moiré Patterns of Twisted Bilayer Transition Metal Dichalcogenides*, Physical Review Letters **121**, 266401 (2018a).
- [61] Sahil Tippireddy, Raju Chetty, Krushna Kumari Raut, Mit H. Naik, Prashanta K. Mukharjee, Manish Jain, R. Nath, Krzysztof Wojciechowski, and Ramesh Chandra Mallik, *Electronic and Thermoelectric properties of Zn and Se double substituted tetrahedrite*, Physical Chemistry Chemical Physics **20**, 28667 (2018a).
- [60] Sudipta Kundu, Satadeep Bhattacharjee, Seung-Cheol Lee, and Manish Jain, *PASTA: Python Algorithms for Searching Transition states*, Computer Physics Communications **233**, 261 (2018).
- [59] Mit H. Naik and Manish Jain, *Substrate screening effects on the quasiparticle band gap and defect charge transition levels in MoS₂*, Physical Review Materials **2**, 084002 (2018b).

- [58] K. S. Vasu, Debabrata Pramanik, Sudipta Kundu, Sridevi S., N. Jayaraman, Manish Jain, Prabal K. Maiti, and A. K. Sood, *Opening of large band gaps in metallic carbon nanotubes by mannose-functionalized dendrimers: experiments and theory*, Journal of Materials Chemistry C **6**, 6483 (2018).
- [57] Indrajit Maity, Prabal K. Maiti, and Manish Jain, *Temperature-dependent layer breathing modes in two-dimensional materials*, Physical Review B **97**, 161406(R) (2018).
- [56] Sahil Tippireddy, Raju Chetty, Mit H. Naik, Manish Jain, Kamanio Chattopadhyay, and Ramesh Chandra Mallik, *Electronic and Thermoelectric Properties of Transition Metal Substituted Tetrahedrites*, The Journal of Physical Chemistry C **122**, 8735 (2018b).
- [55] Mit H. Naik and Manish Jain, *CoFFEE: Corrections For Formation Energy and Eigenvalues for charged defect simulations*, Computer Physics Communications **226**, 114 (2018c).
- [54] Tathagata Biswas, Pramod Ravindra, Eashwer Athresh, Rajeev Ranjan, Sushobhan Avasthi, and Manish Jain, *Optical Properties of $Zn_2Mo_3O_8$: Combination of Theoretical and Experimental Study*, The Journal of Physical Chemistry C **121**, 24766 (2017).
- [53] Dor Gabay, Xueyang Wang, Vitaly Lomakin, Amir Boag, Manish Jain, and Amir Natan, *Size dependent electronic properties of silicon quantum dots – An analysis with hybrid, screened hybrid and local density functional theory*, Computer Physics Communications **221**, 95 (2017).
- [52] Gyan Prakash, Koushik Pal, Manish Jain, U. V. Waghmare, and A. K. Sood, *Origin of the thermal expansion anomaly in layered Bi_2X_3 topological insulators: Ultrafast time-resolved pump-probe experiments and theory*, Physical Review B **96**, 075109 (2017).
- [51] Amogh Kinikar, T Phanindra Sai, Semonti Bhattacharyya, Adhip Agarwala, Tathagata Biswas, Sanjoy K Sarker, HR Krishnamurthy, Manish Jain, Vijay B Shenoy, and Arindam Ghosh, *Quantized edge modes in atomic-scale point contacts in graphene*, Nature Nanotechnology **12**, 564 (2017).
- [50] Mit H. Naik and Manish Jain, *Origin of layer dependence in band structures of two-dimensional materials*, Physical Review B **95**, 165125 (2017).
- [49] Jianyun Zhao, Manisha Thakurathi, Manish Jain, Diptiman Sen, and JK Jain, *Density functional theory of the fractional quantum Hall effect*, Physical Review Letters **118**, 196802 (2017).
- [48] Tathagata Biswas and Manish Jain, *Quasiparticle band structure and optical properties of hexagonal- $YMnO_3$* , Journal of Applied Physics **120**, 155102 (2016).
- [47] Saientan Bag, Manish Jain, and Prabal K. Maiti, *Charge Transport in Dendrimer Melts Using Multiscale Modeling Simulation*, The Journal of Physical Chemistry B **120**, 9142 (2016).

- [46] Nagamalleswararao Dasari, S. R. K. C. Sharma Yamijala, Manish Jain, T. Saha Dasgupta, Juana Moreno, Mark Jarrell, and N. S. Vidhyadhiraja, *First-principles investigation of cubic BaRuO₃: A Hund's metal*, Physical Review B **94**, 085143 (2016).
- [45] Nicholas M. Boffi, Manish Jain, and Amir Natan, *Efficient Computation of the Hartree-Fock Exchange in Real-Space with Projection Operators*, Journal of Chemical Theory and Computation **12**, 3614 (2016a).
- [44] Nicholas M. Boffi, Manish Jain, and Amir Natan, *Asymptotic behavior and interpretation of virtual states: The effects of confinement and of basis sets*, The Journal of Chemical Physics **144**, 084104 (2016b).
- [43] Vidya Kochat, Chandra Sekhar Tiwary, Tathagata Biswas, Gopalakrishnan Ramalingam, Kimberly Hsieh, Kamanio Chattopadhyay, Srinivasan Raghavan, Manish Jain, and Arindam Ghosh, *Magnitude and Origin of Electrical Noise at Individual Grain Boundaries in Graphene*, Nano Letters **16**, 562 (2016).
- [42] Manabendra Kuiri, Chandan Kumar, Biswanath Chakraborty, Satyendra N. Gupta, Mit H. Naik, Manish Jain, A. K. Sood, and Anindya Das, *Probing 2D black phosphorus by quantum capacitance measurements*, Nanotechnology **26**, 485704 (2015).
- [41] R. Chetty, A. Bali, M. H. Naik, G. Rogl, P. Rogl, M. Jain, S. Suwas, and R. C. Mallik, *Thermoelectric properties of Co substituted synthetic tetrahedrite*, Acta Materialia **100**, 266 (2015).
- [40] Sivan Refaely-Abramson, Manish Jain, Sahar Sharifzadeh, Jeffrey B. Neaton, and Leeor Kronik, *Solid-state optical absorption from optimally tuned time-dependent range-separated hybrid density functional theory*, Physical Review B **92**, 081204(R) (2015).
- [39] Atanu Samanta, Manish Jain, and Abhishek K. Singh, *Ultra-sensitive pressure dependence of bandgap of rutile-GeO₂ revealed by many body perturbation theory*, The Journal of Chemical Physics **143**, 064703 (2015).
- [38] Kaustuv Manna, A. K. Bera, Manish Jain, Suja Elizabeth, S. M. Yusuf, and P. S. Anil Kumar, *Structural-modulation-driven spin canting and reentrant glassy magnetic phase in ferromagnetic Lu₂MnNiO₆*, Physical Review B **91**, 224420 (2015).
- [37] Aakanksha Chaudhary, M. Poshit Nag, N. Ravishankar, Tiju Thomas, Manish Jain, and Srinivasan Raghavan, *Synergistic Effect of Mo + Cu Codoping on the Photocatalytic Behavior of Metastable TiO₂ Solid Solutions*, The Journal of Physical Chemistry C **118**, 29788 (2014).
- [36] Manish Jain, Jack Deslippe, Georgy Samsonidze, Marvin L. Cohen, James R. Chelikowsky, and Steven G. Louie, *Improved quasiparticle wave functions and mean field for G₀W₀ calculations: Initialization with the COHSEX operator*, Physical Review B **90**, 115148 (2014).

- [35] Subhamoy Ghatak, Sumanta Mukherjee, Manish Jain, D. D. Sarma, and Arindam Ghosh, *Microscopic origin of low frequency noise in MoS₂ field-effect transistors*, APL Materials **2**, 092515 (2014).
- [34] Andrei Malashevich, Manish Jain, and Steven G. Louie, *First-principles DFT+GW study of oxygen vacancies in rutile TiO₂*, Physical Review B **89**, 075205 (2014).
- [33] Sivan Refaely-Abramson, Sahar Sharifzadeh, Manish Jain, Roi Baer, Jeffrey B. Neaton, and Leeor Kronik, *Gap renormalization of molecular crystals from density-functional theory*, Physical Review B **88**, 081204(R) (2013).
- [32] Jack Deslippe, Georgy Samsonidze, Manish Jain, Marvin L. Cohen, and Steven G. Louie, *Coulomb-hole summations and energies for GW calculations with limited number of empty orbitals: A modified static remainder approach*, Physical Review B **87**, 165124 (2013).
- [31] Johannes Lischner, Jack Deslippe, Manish Jain, and Steven G. Louie, *First-Principles Calculations of Quasiparticle Excitations of Open-Shell Condensed Matter Systems*, Physical Review Letters **109**, 036406 (2012).
- [30] SangKook Choi, Manish Jain, and Steven G. Louie, *Mechanism for optical initialization of spin in NV⁻ center in diamond*, Physical Review B **86**, 041202(R) (2012).
- [29] Jack Deslippe, Georgy Samsonidze, David A. Strubbe, Manish Jain, Marvin L. Cohen, and Steven G. Louie, *BerkeleyGW: A massively parallel computer package for the calculation of the quasiparticle and optical properties of materials and nanostructures*, Computer Physics Communications **183**, 1269 (2012).
- [28] Manish Jain, James R. Chelikowsky, and Steven G. Louie, *Quasiparticle Excitations and Charge Transition Levels of Oxygen Vacancies in Hafnia*, Physical Review Letters **107**, 216803 (2011a).
- [27] Manish Jain, James R. Chelikowsky, and Steven G. Louie, *Reliability of Hybrid Functionals in Predicting Band Gaps*, Physical Review Letters **107**, 216806 (2011b).
- [26] Georgy Samsonidze, Manish Jain, Jack Deslippe, Marvin L. Cohen, and Steven G. Louie, *Simple Approximate Physical Orbitals for GW Quasiparticle Calculations*, Physical Review Letters **107**, 186404 (2011).
- [25] Marie Lopez del Puerto, Manish Jain, and James R. Chelikowsky, *Time-dependent density functional theory calculations for the Stokes shift in hydrogenated silicon clusters*, Physical Review B **81**, 035309 (2010).
- [24] Igor Vasiliev, Marie Lopez del Puerto, Manish Jain, Alejandro Lugo-Solis, and James R. Chelikowsky, *Application of time-dependent density-functional theory to molecules and nanostructures*, Journal of Molecular Structure: THEOCHEM **914**, 115 (2009).
- [23] B. Merheb, P. A. Deymier, K. Muralidharan, J. Bucay, M. Jain, M. Aleshyna-Lesuffleur, R. W. Greger, S. Mohanty, and A. Berker, *Viscoelastic effect on acoustic band gaps in*

- polymer-fluid composites*, Modelling and Simulation in Materials Science and Engineering **17**, 075013 (2009).
- [22] B. Merheb, P. A. Deymier, M. Jain, M. Aleshyna-Lesuffleur, S. Mohanty, A. Berker, and R. W. Greger, *Elastic and viscoelastic effects in rubber/air acoustic band gap structures: A theoretical and experimental study*, Journal of Applied Physics **104**, 064913 (2008).
- [21] Manish Jain, *Structure of Iron-Containing Nitrogenated Carbon*, The Journal of Physical Chemistry C **112**, 9777 (2008).
- [20] M. M. G. Alemany, Manish Jain, Murilo L. Tiago, Yunkai Zhou, Yousef Saad, and James R. Chelikowsky, *Efficient first-principles calculations of the electronic structure of periodic systems*, Computer Physics Communications **177**, 339 (2007).
- [19] Manish Jain, Shih-hung Chou, and Allen Siedle, *In Search for Structure of Active Site in Iron-Based Oxygen Reduction Electrocatalysts*, The Journal of Physical Chemistry B **110**, 4179 (2006).
- [18] Leeor Kronik, Manish Jain, and James R. Chelikowsky, *Electronic structure and spin polarization of MnGaP*, Applied Physics Letters **85**, 2014 (2004).
- [17] M. M. G. Alemany, Manish Jain, Leeor Kronik, and James R. Chelikowsky, *Real-space pseudopotential method for computing the electronic properties of periodic systems*, Physical Review B **69**, 075101 (2004).
- [16] M. Jain and S. P. Gupta, *Formation of intermetallic compounds in the Ni-Al-Si ternary system*, Materials Characterization **51**, 243 (2003).
- [15] W. Russell Burdick, Yousef Saad, Leeor Kronik, Igor Vasiliev, Manish Jain, and James R. Chelikowsky, *Parallel implementation of time-dependent density functional theory*, Computer Physics Communications **156**, 22 (2003).
- [14] Eunjung Ko, Manish Jain, and James R. Chelikowsky, *First principles simulations of SiGe for the liquid and amorphous states*, The Journal of Chemical Physics **117**, 3476 (2002).
- [13] J. C. Woicik, E. J. Nelson, Leeor Kronik, Manish Jain, James R. Chelikowsky, D. Heskett, L. E. Berman, and G. S. Herman, *Hybridization and Bond-Orbital Components in Site-Specific X-Ray Photoelectron Spectra of Rutile TiO₂*, Physical Review Letters **89**, 077401 (2002).
- [12] Leeor Kronik, Manish Jain, and James R. Chelikowsky, *Electronic structure and spin polarization of Mn_xGa_{1-x}N*, Physical Review B **66**, 041203(R) (2002).
- [11] Manish Jain, Vitaliy V. Godlevsky, Jeffrey J. Derby, and James R. Chelikowsky, *First-principles simulations of liquid ZnTe*, Physical Review B **65**, 035212 (2001a).
- [10] Manish Jain, Leeor Kronik, James R. Chelikowsky, and Vitaliy V. Godlevsky, *Electronic structure and spin polarization of Mn-containing dilute magnetic III-V semiconductors*, Physical Review B **64**, 245205 (2001b).

- [9] Leeor Kronik, Igor Vasiliev, Manish Jain, and James R. Chelikowsky, *Ab initio structures and polarizabilities of sodium clusters*, The Journal of Chemical Physics **115**, 4322 (2001).
- [8] J. C. Woicik, E. J. Nelson, T. Kendelewicz, P. Pianetta, Manish Jain, Leeor Kronik, and James R. Chelikowsky, *Partial density of occupied valence states by x-ray standing waves and high-resolution photoelectron spectroscopy*, Physical Review B **63**, 041403(R) (2001).
- [7] Vitaliy V. Godlevsky, Manish Jain, Jeffrey J. Derby, and James R. Chelikowsky, *First-principles calculations of liquid CdTe at temperatures above and below the melting point*, Physical Review B **60**, 8640 (1999).

Conference Proceedings and Book chapters

- [6] D. Gabay, X. Wang, V. Lomakin, A. Boag, M. Jain, and A. Natan, in *2018 International Conference on Electromagnetics in Advanced Applications (ICEAA)* (2018), pp. 210–212. [link].
- [5] David G. O’Neill, Radoslav Atanasoski, Alison K. Schmoedel, George D. Vernstrom, Dennis P. O’Brien, Manish Jain, and Thomas E. Wood, *Vacuum Deposited Non-precious Metal Catalysts for PEM Fuel Cells*, Material Matters **1**, 17 (2006).
- [4] Sanat Mohanty, Gregg Caldwell, Manish Jain, and Cristina U. Thomas, in *Encyclopedia of Chemical Processing*, edited by S. Lee and C. W. LaPierre (Dekker, 2005), chap. 134, pp. 1551–1560. [link].
- [3] James R. Chelikowsky, Manish Jain, and Jeffery J. Derby, in *Computational Modeling and Simulation of Materials (Proceedings of the 10th CIMTEC World Ceramic Congress and Forum on New Materials)*, edited by P. Vincenzini and A. D. Esposito (Techna Group Srl., 2003a), vol. 36, p. 3, ISBN 88-86538-38-3.
- [2] James R. Chelikowsky, Leeor Kronik, Igor Vasiliev, Manish Jain, and Yousef Saad, in *Special Volume, Computational Chemistry*, edited by C. Le Bris (Elsevier, 2003b), vol. 10 of *Handbook of Numerical Analysis*, pp. 613 – 637. [link].
- [1] J. R. Chelikowsky, M. Jain, and J. J. Derby, in *Computer Simulation Studies in Condensed-Matter Physics XV*, edited by David P. Landau, Steven P. Lewis, and Heinz-Bernd Schüttler (Springer Berlin Heidelberg, 2003c), vol. 90 of *Springer Proceedings in Physics*, pp. 149–162, ISBN 978-3-642-55522-0. [link].

Patents

- [3] Ali Berker, Richard W Greger, Manish Jain, Marie Alshohna Ep Lesuffleur, and Sanat Mohanty, *Sound barrier for audible acoustic frequency management* (2012), US Patent 8,132,643.
- [2] Ali Berker, Manish Jain, Mark D Purgett, Sanat Mohanty, Pierre A Deymier, and Bassam Merheb, *Viscoelastic phononic crystal* (2016), US Patent 9,324,312.

- [1] Raghunath Padiyath, Marc D Radcliffe, Cristina U Thomas, Charles A Marttila, Manish Jain, Michael F Weber, and Feng Bai, *Infrared light reflecting film* (2010), US Patent 7,652,736.

Presentations

Invited Talks

- [38] Imaging Facility seminar at the Molecular Foundry, Berkeley, USA, March 2020.
- [37] Novel Phases of Quantum Matter, Bangalore, January 2020.
- [36] International Workshop on Advances in 2D Materials, Trivandrum, July 2019.
- [35] Nano India 2019, Kottayam, April 2019.
- [34] First Indian Materials Conclave and 30th Annual General Meeting of Materials Research Society of India, Bangalore, February 2019.
- [33] Recent trends in Condensed Matter Research, Kothamangalam, January 2019.
- [32] 10th APCTP-IACS-KIAS Conference on Novel oxide materials and low dimensional systems, Seoul, South Korea, October 2018.
- [31] Modelling and Simulations of Materials for Energy and the Environment, Bangalore, December 2018.
- [30] Planning the next generation of Electronic structure codes, Austin, USA, November 2018.
- [29] Indian Institute of Science – Nanyang Technological University Workshop, Bangalore, September 2018.
- [28] Evolution of Electronic Structure Theory and Experimental Realization, Chennai, September 2018.
- [27] Computational methods in physics and chemistry, Manipal, August 2018.
- [26] National Conference on Quantum Condensed Matter, Mohali, July 2018.
- [25] Practical Quantum Mechanics for Electronic Materials, Austin, USA, June 2018.
- [24] Emergent Phenomena in Classical and Quantum Systems, Kolkata, February 2018.
- [23] Recent Advances in Molecular Simulations, Bangalore, February 2018.
- [22] 9th IACS-APCTP Conference on Novel oxide materials and low dimensional systems, Kolkata, December 2017.
- [21] National Institute of Science Education and Research, Bhubaneswar, September 2017.
- [20] 18th Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, Luxembourg, January 2016.

- [19] DFT and TDDFT in the real-space formalism within the PARSEC code: perspectives and future development, Tel Aviv, Israel, December 2015.
- [18] 7th IACS-APCTP-Academy Conference on Novel oxide materials and low dimensional systems, Coorg, December 2015.
- [17] Indian Institute of Science Education and Research, Bhopal, April 2015.
- [16] Department of Chemical Engineering, Indian Institute of Science, Bangalore, March 2015.
- [15] Current Trends in Condensed Matter Physics, February 2015.
- [14] Winter School on Materials and Processes for Energy and Environment, Bangalore, January 2015.
- [13] Cambridge-JNCASR Winter School on Frontiers in Materials Science, Bangalore, December 2014.
- [12] Materials Simulations Theory and Numerics, Summer school, Pune, June-July 2014.
- [11] Physics and Chemistry of Materials : Computation and Experiments, Kolkata, February 2014.
- [10] International Union of Materials Research Societies – International Conference in Asia 2013, Bangalore, December 2013.
- [9] 5th IACS-IISc-APCTP Conference on Novel oxide materials and low dimensional systems, Bangalore, December 2013.
- [8] Numerical Many Body Methods in Quantum Chemistry and Physics, Coorg, December 2013.
- [7] IBM, Bangalore, October 2013.
- [6] Center for Nano Science and Engineering, Indian Institute of Science, Bangalore, April 2013.
- [5] Indian Institute of Science, Indian Institute of Science Education and Research (Pune and Mohali), Jawaharlal Nehru Center for Advanced Scientific Research, National Chemical Laboratory, Tata Insitute for Fundamental Research, Indian Institute of Technology (Kanpur), May 2012.
- [4] EFRC:CST Density Functional Theory Meeting, Santa Fe, May 2010.
- [3] Workshop on Computational Materials and Molecular Electronics, Austin, October 2005.
- [2] Central Scientific Instruments Organization, Chandigarh, India, May 2002.
- [1] University of Illinois, Chicago, November 2001.