

Mit H. Naik

Curriculum Vitae

Contact Information

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Summary

As an experienced computational physicist with a strong background in theory, my expertise lies in quantum mechanics-based methods such as density functional theory and many-body perturbation theory (GW-BSE). I have a demonstrated track record of achievement in condensed matter physics, as well as a solid foundation in applied mathematics and algorithm development. My research is published in 24 peer-reviewed articles, including first-author publications in *Nature*, *Science*, *Nature Materials* and *Physical Review Letters*. I have been invited to present my research at the top conferences in my field such as APS March Meeting, MRS Fall Meeting and the Electronic Structure Workshop. I was awarded a medal for the best PhD thesis. **Total Citations:** 1140, **h-index:** 14 (source: [Google Scholar](#))

Research accomplishments

In my doctoral research, we were the first to demonstrate that 2D transition metal dichalcogenide (TMD) based moiré superlattices undergo substantial structural transformations and can accommodate electronic flat bands. What set this discovery apart was the revelation that TMDs lacked the concept of "magic" twist-angles, a characteristic well-documented in the context of twisted bilayer graphene; essentially offering an easily accessible pathway to harness strong correlations. We also studied intrinsic sulfur vacancy defects in monolayer MoS₂, offering fundamental insights into substrate screening effects on charged defect levels. During my postdoc, I developed the pristine unit-cell matrix projection (PUMP) approach, using which we were able to perform first principles GW-BSE calculations on a record breaking 4000 atom moiré unit-cell, resulting in the discovery of an intralayer charge-transfer exciton, featuring photoexcited electron and hole separation within a single layer of a 2D material. This discovery fundamentally reshaped our understanding of moiré excitons by challenging the prevailing continuum model, which had been the sole theoretical framework for understanding moiré excitons. Working closely with experimentalists, we were able to validate several predictions from my calculations on different moiré superlattices using doping-dependent reflection contrast spectroscopy, scanning transmission electron energy loss spectroscopy, and scanning tunnelling spectroscopy.

Education

Postdoctoral scholar, 12/2019 – present
[Louie research group](#), Department of Physics,
University of California, Berkeley

Adviser: Prof. Steven G. Louie

Visiting Student Researcher, 10/2019-12/2019

Louie research group, Department of Physics,
University of California, Berkeley

PhD, Theoretical condensed matter physics, 11/2019

Quantum theory of materials group,

Department of Physics, Indian Institute of Science, Bangalore, India

Thesis title: “*Taming Electrons in 2D Materials: Influence of Substrates, Defects and Moiré Superlattices*”. Adviser: Prof. Manish Jain

M.S., Physics, 08/2014, Department of Physics, Indian Institute of Science
Bangalore, India

Awards

Winner of lightning talk challenge at the department of energy’s EFRC-Hub-CMS-CCS PI Meeting, 2023

Kumari L A Meera Memorial Medal awarded for best PhD thesis in the Department of Physical Sciences, Indian Institute of Science, 2021

Best oral presentation award at “Winter school on frontiers in materials science”, JNCASR, Bangalore, India, 2017

News articles and podcasts about my research

- News article “New quasiparticle discovered in moiré patterns”, published by 10 news outlets.
- Supersized science podcast with Jorge Salazar on our *Nature* paper about intralayer charge transfer moiré excitons.
- Berkeley Lab news center article on our *Science* paper imaging the spatial extent of a moiré exciton.

Teaching experience

- Taught 6 lectures for a graduate level solid state physics course at UC Berkeley acting as a substitute for my postdoc advisor.
- Teaching assistant of graduate level computational physics course for two years.

Publications

Full list of articles: [Google scholar](#)

First author articles:

- [10] Hongyuan Li*, Ziyu Xiang*, **Mit H. Naik***, Woochang Kim, Zhenglu Li, Renee Sailus, Rounak Banerjee, Takashi Taniguchi, Kenji Watanabe, Sefaattin Tongay, Alex Zettl, Felipe H. da Jornada, Steven G. Louie, Michael F. Crommie and Feng Wang, *Imaging Moiré Excited States with Photocurrent Tunneling Microscopy*, Nature Materials, in press (2023)
- [9] Sandhya Susarla*, **Mit H Naik***, Daria D Blach, Jonas Zipfel, Takashi Taniguchi, Kenji Watanabe, Libai Huang, Ramamoorthy Ramesh, Felipe H da Jornada, Steven G Louie, Peter Ercius, Archana Raja, *Hyperspectral imaging of excitons within a moiré unit-cell with a sub-nanometer electron probe*, Science, 378, 6625, 1235-1239 (2022)
- [8] **Mit H. Naik***, Emma C. Regan*, Zuocheng Zhang*, Yang-hao Chan, Zhenglu Li, Danqing Wang, Yoseob Yoon, Chin Shen Ong, Wenyu Zhao, Sihan Zhao, M. Iqbal Bakti Utama, Beini Gao, Xin Wei, Mohammed Sayyad, Kentaro Yumigeta, Kenji Watanabe, Takashi Taniguchi, Sefaattin Tongay, Felipe H. da Jornada, Feng Wang and Steven G. Louie, *Nature of novel moiré exciton states in WSe₂/WS₂ heterobilayers*, Nature 609, pages 52–57 (2022)
- [7] Hongyuan Li*, Shaowei Li*, **Mit H. Naik***, Jingxu Xie, Xinyu Li, Jiayin Wang, Emma Regan, Danqing Wang, Wenyu Zhao, Sihan Zhao, Salman Kahn, Kentaro Yumigeta, Mark Blei, Takashi Taniguchi, Kenji Watanabe, Sefaattin Tongay, Alex Zettl, Steven G. Louie, Feng Wang and Michael F. Crommie, *Imaging moiré flat bands in three-dimensional reconstructed WSe₂/WS₂ superlattices*, Nature Materials, 20, 945–950 (2021)
- [6] **Mit H. Naik**, Sudipta Kundu, Indrajit Maity, and Manish Jain, *Origin and Evolution of Ultraflatbands in Twisted Bilayer Transition Metal Dichalcogenides: Realization of Triangular Quantum Dots*, Phys. Rev. B 102, 075413 (2020)
- [5] **Mit H. Naik**, Indrajit Maity, Prabal K. Maiti, and Manish Jain, *KolmogorovCrespi Potential For Multilayer Transition-Metal Dichalcogenides: Capturing Structural Transformations in Moir Superlattices*, The Journal of Physical Chemistry C 123, 9770 (2019).
- [4] **Mit H. Naik** and Manish Jain, *Ultraflatbands and Shear Solitons in Moiré Patterns of Twisted Bilayer Transition Metal Dichalcogenides*, Phys. Rev. Lett. 121, 266401 (2018).
- [3] **Mit H. Naik** and Manish Jain, *Substrate screening effects on the quasiparticle band gap and defect charge transition levels in MoS₂*, Phys. Rev. Materials 2, 084002 (2018).

[2] **Mit H. Naik** and Manish Jain, *CoFFEE: Corrections For Formation Energy and Eigenvalues for charged defect simulations*, Computer Physics Communications 226, 114 (2018)

[1] **Mit H. Naik** and Manish Jain, *Origin of layer dependence in band structures of two-dimensional materials*, Phys. Rev. B 95, 165125 (2017).

*: Equal contribution

Other articles:

[15] Chen Hu, **Mit H. Naik**, Yang-hao Chan and Steven G. Louie, *Excitonic interactions and mechanism for ultrafast interlayer photoexcited response in van der Waals heterostructures*, arXiv:2305.17335 (2023)

[14] Yang-hao Chan, Jonah B. Haber, **Mit H. Naik**, Jeffrey B. Neaton, Diana Y. Qiu, Felipe H. da Jornada, and Steven G. Louie, *Exciton Lifetime and Optical Line Width Profile via Exciton-Phonon Interactions: Theory and First-Principles Calculations for Monolayer MoS₂*, Nano Letters 23, 9, 3971–3977 (2023)

[13] Sudipta Kundu, **Mit H. Naik**, H. R. Krishnamurthy, and Manish Jain, *Moiré induced topology and flat bands in twisted bilayer WSe₂: A first-principles study*, Phys. Rev. B 105, L081108 (2022)

[12] Hongyuan Li, Shaowei Li, **Mit H. Naik**, Jingxu Xie, Xinyu Li, Emma Regan, Danqing Wang, Wenyu Zhao, Kentaro Yumigeta, Mark Blei, Takashi Taniguchi, Kenji Watanabe, Sefaattin Tongay, Alex Zettl, Steven G. Louie, Michael F. Crommie, and Feng Wang, *Imaging local discharge cascades for correlated electrons in WS₂/WSe₂ moiré superlattices*, Nature Physics 17, pages 1114–1119 (2021)

[11] Saimit Naik, **Mit H. Naik**, Indrajit Maity and Manish Jain, *TWISTER: Construction and structural relaxation of commensurate moiré superlattices*, Computer Physics Communications, 271, 108184 (2021)

[10] Indrajit Maity, **Mit H. Naik**, Prabal K. Maiti, H. R. Krishnamurthy and Manish Jain, *Phonons in twisted transition-metal dichalcogenide bilayers: Ultrasoft phonons and a transition from a superlubric to a pinned phase*, Phys. Rev. Research 2, 013335 (2020)

[9] Sudipta Kundu, **Mit H. Naik**, and Manish Jain, *DFT+GW Study of Charge Transition Levels of Point Defects in Mono and Bi-layer Phosphorene*, Phys. Rev. Materials 4, 054004 (2020).

[8] S. Nayak, **Mit H. Naik**, M. Jain, U. V. Waghmare, and S. M. Shivaprasad, *First-principles theoretical analysis and electron energy loss spectroscopy of vacancy defects in bulk and*

nonpolar (1010) surface of GaN, Journal of Vacuum Science & Technology A 38, 063205 (2020)

- [7] Anomitra Sil, Devendra S. Negi, **Mit H. Naik**, Manish Jain, Ranjan Datta, Rajeev Ranjan, and P. S. Anil Kumar, *Large intrinsic magnetization in an epitaxial BiFeO₃/NdGaO₃ system*, EPL (Europhysics Letters) 126, 57003 (2019).
- [6] Tanweer Ahmed, **Mit H. Naik**, Simran Kumari, Smriti P. Suman, Rahul Debnath, Sudipta Dutta, Umesh Waghmare, Manish Jain, Arindam Ghosh, and Manish Jain, *Thermodynamically stable octahedral MoS₂ in van der Waals hetero-bilayers*, 2D Materials (Accepted) (2019).
- [5] 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*, Phys. Chem. Chem. Phys. 20, 28667 (2018).
- [4] 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 (2018).
- [3] Anomitra Sil, **Mit H. Naik**, Rajeev Ranjan, and P. S. Anil Kumar, *Tuning the crystallographic orientation and magnetic properties of multiferroic CuO epitaxial film on single crystalline SrTiO₃ substrates*, Journal of Applied Physics 124, 085303 (2018).
- [2] 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).
- [1] 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).

Presentations

- [17] Lightning talk: “Diverse Nature of Excitonic States in Transition Metal Dichalcogenide Moiré Superlattices”, EFRC-Hubs-CMS-CCS Virtual PI Meeting
- [16] Invited talk: “Bethe Salpeter equation calculations in moiré superlattices with thousands of atoms in the unit-cell“, Electronic Structure Workshop, Merced, 2023
- [15] Invited talk: “Diverse Nature of Excitonic States in Transition Metal Dichalcogenide Moiré Superlattices“, APS March Meeting 2023
- [14] Invited talk: “Diverse Nature of Excitonic States in Transition Metal Dichalcogenide Moiré Superlattices“, MRS Fall Meeting and Exhibit 2022

- [13] Conference talk: "Making the intractable tractable: GW-BSE calculation of the nature of interlayer and intralayer moiré excitons in large-area moiré superlattices", APS March Meeting 2022
- [12] Conference talk: "Intralayer moiré exciton states in transition metal dichalcogenide heterostructures: a GW-BSE study", APS March Meeting 2021
- [11] Invited seminar: "Nature of novel moiré exciton states in transition metal dichalcogenide heterostructures", Molecular Foundry, Lawrence Berkeley Lab, 2021
- [10] Invited talk: "Origin and nature of moiré excitons in twisted bilayer transition metal dichalcogenides", C2SEP/EM Scientific Advisory Board meeting, 2021
- [9] Invited talk: "Moiré excitons in twisted bilayer TMD heterostructures: a first-principles GW-BSE study", 2nd Berkeley Excited States Conference, 2021
- [8] Conference talk: "Ultraflat bands and shear solitons in Moiré patterns of twisted bilayer transition metal dichalcogenides", APS March meeting 2019
- [7] Invited seminar: "Taming electrons in 2D materials: influence of substrates, defects and moiré superlattices", Lawrence Berkeley National Lab, Berkeley, 2018
- [6] Conference talk: "Ultraflatbands and Shear Solitons in Moiré Patterns of Twisted Bilayer Transition Metal Dichalcogenides", XXX IUPAP Conference on Computational Physics, University of California, Davis, 2018.
- [5] Seminar: "Taming electrons in 2D materials: influence of substrates, defects and moiré superlattices", University of Luxembourg, 2018
- [4] Conference talk: "CoFFEE: Corrections For Formation Energy and Eigenvalues for charged defect simulations", Conference on Physics of Defects in Solids: Quantum Mechanics Meets Topology, International Centre for Theoretical Physics, Trieste, Italy, 2018
- [3] Seminar: "Taming electrons in 2D materials: influence of substrates, defects and moire superlattices", Ecole Polytechnique Federale de Lausanne (EPFL), 2018
- [2] Talk: "Substrate screening effects on the quasiparticle band gap and defect charge transition levels in MoS₂", Winter school on frontiers in materials science, JNCASR, Bangalore, India, 2017.
- [1] Poster: "Origin of layer dependence in band structures of two-dimensional materials", Workshop on spectroscopy and dynamics of photo induced electronic excitations, International Centre for Theoretical Physics, Trieste, Italy, 2017.