Priya Mahadevan

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Guidance of Students/Post-Docs/Scientists

a) Ph.D. Students

1. Joydeep Chatterjee; Electronic and structural properties of Semiconductor Heterostructures; Under progress
2. Sumanti Patra; Electronic structure of twisted bilayers of transition metal dichalcogenides; Under progress
3. Debayan Mondal; Electronic structure of htbrid perovskites; Under progress
4. Prasun Boyal; Spin orbit effects in transition metal dichalcogenides; Under progress
5. Shivam Mishra; Electronic structure of semiconductor nanoplatelets; Under progress
6. Krishnendu Patra; Metal insulator transitions in transition metal compounds; Under progress
7. Shinjini Paul; Electronic structure of ultrathin films of transition metal oxides; Under progress

b) Post-Docs

1. Priyanka Garg; Properties of hybrid perovskites

Publications

a) In journals

1. Sumanti Patra, Poonam Kumari, and **Priya Mahadevan**, *Evolution of the electronic structure of twisted bilayer $MoSe_2$*, Physical Review B, 102, 205415, 2020
2. Shishir K. Pandey, Ruma Das, and **Priya Mahadevan**, *Layer-Dependent Electronic Structure Changes in Transition Metal Dichalcogenides: The Microscopic Origin*, ACS Omega, 5, 15169–15176, 2020
3. Indrani Kar, Joydeep Chatterjee, Luminita Harnagea, Y. Kushnirenko, A. V. Fedorov, Deepika Shrivastava, B. Büchner, **P. Mahadevan** and **S. Thirupathaiah**, *Metal-chalcogen bond-length induced electronic phase transition from semiconductor to topological semimetal in ZrX_2 (X = Se and Te)*, Physical review B, 101, 165122, 2020

Talks / Seminars Delivered in reputed conference / institutions

1. Talk at APS March Meeting 2021; Mar 19, 2021; Americal Physical Society Meeting; 5days
2. Invited talk at National Conference on Quantum Matter Heterostructure; Feb 18, 2021; IIT Roorkee and INST Mohali; 3 days
3. Invited talk at National Level Lecture Workshop in Fronteirs in Science and Engineering by Women in Science; Feb 6, 2021; Deen Dayal Upadhyay College; 15 days
4. Talk at CMD2020GEFES; Sep 4, 2020; European Physical Society; 3 days

Administrative duties

1. Associate Dean Academic Programme till Dec 2020

2. Head of the Department, Condensed Matter Physics and Material Science
3. Members of various DST/SERB appointed review committees
4. Members of various internal committees

Awards, Recognitions

1. SERB Power fellow (2021-2024)
2. Editorial Advisory Board Member, ACS Energy Letters (2021-2022).
3. Editorial Advisory Board Member, Journal of Magnetism and Magnetic Materials (2021-2025)

Membership of Learned Societies

1. American Physical Society (since November 2020)

Extramural Projects (DST, CSIR, DAE, UNDP, etc.)

1. Ab-initio search for topological Mott insulators; DST International Division; 2021-2023; PI
2. Twistronics with transition metal dichalcogenides; SERB -IRPHA; 2020-2025; PI
3. Electronic, structural and optical properties of semiconductor nanoplatelets; DST Nanomission; 2019-2021; PI

Outreach program organized / participated

1. Speaker at outreach programme in Oxford College of Science, Bangalore, January 2021 for college students
2. Speaker at Short Term Training Programme on Emerging Trends in Research and Innovation - Tips and Techniques, SVNIT Surat, January (2021) for college students.
3. Speaker at Emerging Trends in Research Methodology in Condensed Matter, Materials Science and Nanoscience 2020, December (2020) for college students

Areas of Research

Optical properties, electronic structure, magnetism

Recently twisted bilayers of Mo and W based transition metal dichalcogenides have been found to behave like strongly correlated materials, exhibiting wigner crystal formation, semiconductor-metal-semiconductor transitions, zero resistance states on hole doping etc. We have re-examined the electronic structure of twisted bilayers of MoSe2 considering certain angles that lead to large commensurate unit cells. The unit cells we generate contain around 1500 or larger number of atoms while the primitive cell contains just 6 atoms. Consequently, one would expect no dispersional width for the bands here, with all bands folding back to a significantly small Brillouin zone. This has been the understanding of the formation of flatbands and the associated correlated electron physics that one finds. If one examined the untwisted limit, one finds small modifications in the band structure of the bilayer with respect to the monolayer. For the twisted structures, in the limit of weak perturbation one expects the untwisted or unperturbed limit to be largely retained. Therefore a measure of the perturbation with respect to the untwisted limit could help us understand the modifications in the electronic structure. With this aim, we projected the perturbed eigen functions onto the untwisted eigenfunctions. The latter represent the unperturbed limit. The effect of the perturbing potential would be to scatter the electrons into a different momentum state connected by a reciprocal lattice vector. Angles of rotation were considered so that they led to two similar sized cells. Surprisingly, one found that the low lying electronic structure for the large twist angle was very similar to the unperturbed primitive cell results. This implied that the low energy electronic structure for the large twist angles could be described by the unrotated limit, and most importantly flat bands were not a consequence of the large moire cell involved. Considering a smaller angle of 3.48 degrees, one found the emergence of bands which were localized both in real space as well as k-space, leading to split off bands. These were not restricted to only this choice of twist angle, but were found for other angles in the range 2-6 degrees also. Examining the origin of the flat band formation, we find that correlated bond disorder emerging from large patches where the interlayer interaction strengths

(perturbation) are larger is responsible for the flat band formation. This appeared in Phys. Rev. B **102**, 205415 (2020).

We have examined the electronic structure evolution with thickness in transition metal dichalcogenides MX2, where M = Mo,W and X = S,Se and Te. These are generally referred to as van der Waals materials on the one hand, yet one has band gap changes as large as 0.6 eV with thickness in some instances. This does not seem to be consistent with a description where the dominant interactions are van der Waals interactions. Mapping onto a tight binding model allows us to quantify the electronic structure changes which are found to be dictated solely by interlayer hopping interactions. This has appeared in ACS Omega **5**, 15169 (2020).

Plan of Future Work Including Project

1. The model that we have proposed to understand the properties of twisted bilayers of transition metal dichalcogenides will be extended to other transition metal dichalcogenides to examine the implications of a split off band formation there and its tunability under different external conditions. The relevant tight-binding model will be constructed to examine various features of the twisted bilayers beyond the purview of the ab-initio calculations. Our earlier work has shown the importance of interlayer coupling in determining the electronic structure evolution as a function of the number of layers. We are working on an effective low energy model to capture these trends. This will then be used to calculate the optical spectra as a function of the number of layers.