CMD30-FisMat2023

Two-Dimensional Excitonic Insulators

4-8 September 2023, Politecnico Milan, Italy

Organised by
Hope Bretscher, MPI, Germany
Elisa Molinari, Univ Modena, Italy
Massimo Rontani, Cnr-Nano, Italy

The research on **excitonic insulators** has its origin in a heretic prediction formulated more than 50 years ago by a group of visionary physicists, including Leonid Keldysh and Walter Kohn: If a narrow-gap semiconductor, or a semimetal with slightly overlapping conduction and valence bands, failed to fully screen its intrinsic charge carriers, then excitons - electron-hole pairs bound together by Coulomb attraction - would spontaneously form. This would destabilize the ground state, leading to a reconstructed 'excitonic insulator' - a condensate of excitons at thermodynamic equilibrium. This chimeric phase shares fascinating similarities with the Bardeen-Cooper-Schrieffer superconductor: a distinctive broken symmetry, inherited by the exciton character, and collective modes of purely electronic origin. Its observation was deterred for many decades by the trade-off between competing effects in the semiconductor: as the size of the energy gap decreases, favoring spontaneous exciton generation, the screening of the electron-hole interaction increases, suppressing the exciton binding energy.

In the last two years, mounting evidence has been accumulating in 2d materials, as they combine optimal band structures, poor screening behavior, truly long-ranged interactions, and giant excitonic effects. New electron-hole bilayers hold promise of room-temperature superfluid behavior [1-4], whereas signatures of the long-sought bulk phase were found in monolayers [5-7]. Excitonic materials exhibit other kinds of order as well: a variety that includes topological insulators [6-8], ferroelectrics [8,9], unconventional superconductors [6-7,9], often depending on tiny variations of tunable parameters, such as doping, pressure, strain. This introduces new urgent and far-reaching questions, concerning the role of excitonic correlations in a plethora of allegedly unrelated phenomena, whose interplay is just beginning to be explored. At the same time, the long-term challenge of establishing the excitonic insulator through the signatures of macroscopic quantum coherence is attracting renewed interest in this class of materials.

By collecting the key actors of theoretical and experimental research, who are spread among different communities, this MiniColloquium aims at in-depth analysis of common themes and novel challenges, to progress our understanding of interacting systems in low dimensions.

The **MiniColloquium Two-Dimensional Excitonic Insulators** is partially funded by
MUR PRIN2017 No. 2017BZPKSZ "EXC-INS"

References:

[1] Liu, X. et al. Crossover between strongly coupled and weakly coupled exciton superfluids. Science 375, 205-209 (2022). https://www.science.org/doi/10.1126/science.abg1110

[2] Ma, L. et al. Strongly correlated excitonic insulator in atomic double layers. Nature 598, 585-589 (2021). https://www.nature.com/articles/s41586-021-03947-9

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[5] Bretscher, H. et al. Imaging the coherent propagation of collective modes in the excitonic insulator Ta2NiSe5 at room temperature. Science Adv. 7, eabd6147 (2021). https://www.science.org/doi/10.1126/science.abg1110

[6] Jia, Y. et al. Evidence for a monolayer excitonic insulator. Nature Phys. 18, 87–93 (2022). https://www.nature.com/articles/s41567-021-01422-w

[7] Sun, B. et al. Evidence for equilibrium exciton condensation in monolayer WTe2. Nature Phys. 18, 94–99 (2022). https://www.nature.com/articles/s41567-021-01427-5

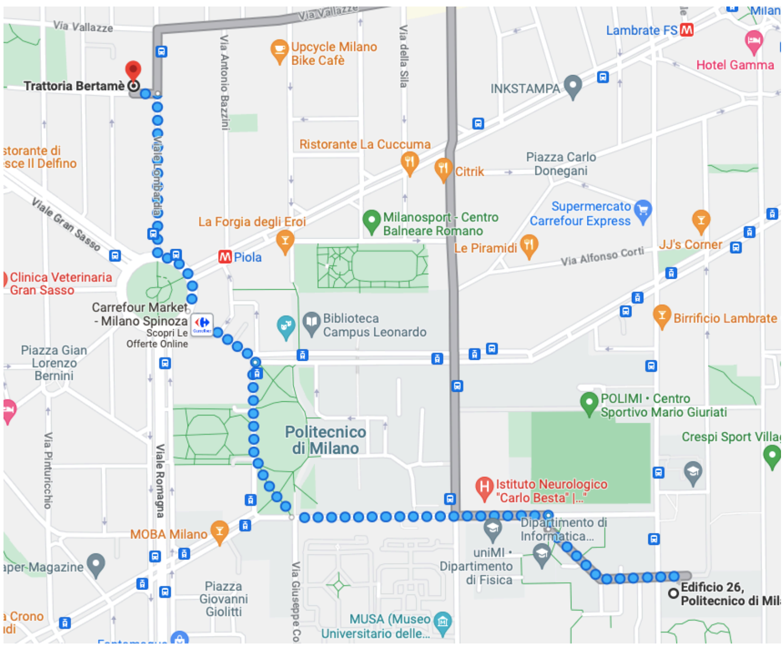
[8] Varsano, D. et al. A monolayer transition-metal dichalcogenide as a topological excitonic insulator. Nature Nanotech. 15, 367–372 (2020). https://www.nature.com/articles/s41565-020-0650-4

[9] Ataei, S. et al. Evidence of ideal excitonic insulator in bulk MoS2 under pressure. PNAS 118, e2010110118 (2021). https://www.pnas.org/doi/abs/10.1073/pnas.2010110118

Venue:

The Two dimensional excitonic insulators MiniColloquium will take place in the building 26 of the Politecnico di Milano.

The Minicolloquium dinner will be held at Trattoria Bertamè, Via Francesco Lomonaco, 13b, 20131 Milano MI, Italia.



CMD30-FisMat2023 – Two dimensional excitonic insulators

Program

4-8 September 2023, Politecnico Milan, Italy

Monday 4 September (room 26.1.5.)

Session I Chair: Elisa Molinari

15.15 – 15.30	**Hope Bretscher, Elisa Molinari, Massimo Rontani** ***Welcome address & overview***
15.30 – 16.00	**David Cobden (invited)** *Peculiar behavior in two-dimensional semimetals such as WTe2*
16.00 – 16.15	**Daniele Varsano** *Theory of the excitonic insulator phase in monolayer WTe2*
16.15 – 16.30	**Michael S. Fuhrer** *Origin of spatial modulations of the local density of states in WTe2*
16.30 – 16.45	**Claudia Cardoso** *Anomalous plasmon dispersion in topological semimetals*
16.45 – 17.00	**Andrea Blason** *Exciton topology and condensation in a model quantum spin Hall insulator*
17.00 – 17.15	**Francois Dubin** *From Mott insulators to checkerboard solids with dipolar excitons*
17.15 – 17.30	**Sara Conti** *Chester supersolid of excitons in semiconductor heterostructures*
17.30 – 17.45	**Igor Bondarev** *Magnetic-field-induced Wigner crystallization of charged interlayer excitons in van der Waals heterostructures*

Monday 4 September (poster room)

Happy Hour and Poster Session

17.45	**Giacomo Sesti** *Excitonic insulator phase in narrow-gap carbon nanotubes*
17.45	**Alperen Tugen** *Optical detection of excitonic insulators in van der Waals heterobilayers: Progress and future prospects*

Tuesday 5 September (room 26.1.5.)

Session II   Chair: Hope Bretscher

10.45 – 11.00	**Philip Kim** *Transport signature of magnetoexciton insulating state in electron-hole graphene double-layers*
11.00 – 11.15	**Filippo Pascucci** *Josephson effect and superfluidity in exciton heterobilayers*
11.15 – 11.30	**Fredrik Nilsson** *Ab initio predictions of new exciton insulators*
11.30 – 11.45	**Youngwook Kim** *Quantum Hall superfluid in twisted bilayer/double bilayer graphene*
11.45 – 12.00	**Peter Littlewood** *Non reciprocal phase transitions in polaritonic systems*
12.00 – 12.15	**Matteo D'Alessio** *Excitons in bilayer* WTe_2
12.15 – 12.30	**Friedhelm Bechstedt** *Can Xenes be excitonic insulators?*
12.30 – 12.45	**Miki Bonacci** *Possible excitonic instability in* $AsCuLi_2$
12.45 – 13.00	**Yuanchang Li** *Materials design of magnetic and topological excitonic insulators from first-principles*
13.00 – 13.15	**Huaiyuan Yang** *Spin-triplet topological excitonic insulators in two-dimensional materials*

Tuesday 5 September (room 26.1.5.)

Session III Chair: Massimo Rontani

15.15 – 15.30	**Girsh Blumberg** *Is Ta_2NiSe_5 a true excitonic insulator?*
15.30 – 15.45	**Denis Golez** *Symmetries and collective mode in excitonic insulators*
15.45 – 16.00	**Satoshi Ejima** *Order, criticality, and excitations in the extended Falicov-Kimball model:* *A case study for the strong excitonic insulator candidate Ta_2NiSe_5*
16.00 – 16.15	**Banhi Chatterjee** *Ground state symmetries and collective modes in Ta_2NiSe_5 - an excitonic insulator candidate*
16.15 – 16.30	**Yuelin Shao** *Electrical breakdown of excitonic insulators*
16.30 – 16.45	**Giacomo Sesti** *Excitonic vs Mott insulator in carbon nanotubes: A proposed experimental test*
16.45 – 17.00	**Giacomo Mazza** *Hidden excitonic quantum states with broken time reversal symmetry*
17.00 – 17.45	**Discussion Session I** Moderator: Philip Kim
19.30	**MiniColloquium Dinner:** Trattoria Bertamè, Via Francesco Lomonaco, 13b, 20131 Milano MI, Italia

Wednesday 6 September (room 26.1.5.)

Session IV Chair: Elisa Molinari

15.15 – 15.30	Abstract Withdrawn
15.30 – 15.45	**Lorenzo Del Re** *Correlated phases in AB-stacked twisted TMD bilayers*
15.45 – 16.00	**Sufei Shi** *Excitonic insulator in a Bilayer WSe2/monolayer WS2 moiré superlattice*
16.00 – 16.15	**Ivan Amelio** *Polaron spectroscopy of a bilayer excitonic insulator*
16.15 – 16.30	**Adriano Amaricci** *Strongly correlated exciton-polarons in twisted homobilayer of transition metal dichalcogenides*
16.30 – 16.45	**Fulvio Paleari** *Bulk MoS2 under pressure as an excitonic insulator*
16.45 – 17.00	**Benjamin Remez** *Theory of disordered excitonic insulators*
17.00 – 17.45	**Discussion Session II**

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Abstracts

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Strongly correlated exciton-polarons in twisted homobilayer of transition metal dichalcogenides

Adriano Amaricci[1], Giacomo Mazza[2]

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[2]Dipartimento di Fisica, Università di Pisa, Italy

We consider dressing of excitonic properties by strongly correlated electrons in gate-controlled twisted homobilayer heterostructures. The combined effect of the moiré potential and the Coulomb interaction supports the formation of different strongly correlated phases depending on the filling, including charge-ordered metals or incompressible insulators at integer occupation. The coupling between excitons and electrons results in a splitting of the excitonic resonance into an attractive and a repulsive polaron peak. Analyzing the properties of the exciton-polarons across the different phases of the system, we reveal a discontinuous evolution of the spectrum with the formation of a double-peak structure in the repulsive polaron branch. The double-peak structure emerges for noninteger fillings and it is controlled by the energy separation between the quasiparticle states close to the Fermi level and the high-energy doublons excitations. Our results demonstrate that exciton-polarons carry a clear hallmark of the electronic correlations and, thus, provide a direct signature of the formation of correlation-driven insulators in gate-controlled heterostructures.

Polaron spectroscopy of a bilayer excitonic insulator

Ivan Amelio[1], Neil Drummond[2], Eugene Demler[3], Richard Schmidt[4], Atac Imamoglu[5]

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[2]Department of Physics, Lancaster University, United Kingdom
[3]Institute for Theoretical Physics, ETH Zurich, Switzerland
[4]Institut fur Theoretische Physik, Universitaet Heidelberg, Germany
[5]Institute of Quantum Electronics ETH Zurich, Switzerland

A recent experiment by the Cornell group suggests that a ground-state excitonic insulator, in which interlayer pairing of electron and holes develops, has been achieved using heterostructures of two-dimensional materials. In our recent proposal [arXiv:2210.03658] we show that polaron spectroscopy, a tool which has already been useful in probing other many-body states in two-dimensional materials (Wigner crystals, anomalous Hall effect, Mott states etc.), yields further insight on the nature of the excitonic insulator. In particular, we analyze a scheme where an optically generated intralayer exciton is screened by excitations out of the excitonic insulator to form interlayer polarons. Simulating 4-body systems with Quantum Monte-Carlo, we first determine the binding energy of the biexciton state composed of inter- and intralayer excitons, which plays a central role in understanding polaron formation. We describe the excitations out of the ground-state condensate using BCS theory and use a single interacting-quasiparticle-pair excitation Ansatz to describe dynamical screening of optical excitations. This technique allows to interpolate between the Bose regime at small interlayer distance and density, where the ground states excitons are tighly bound, and the BCS regime at large distance and density. In the BCS regime the oscillator strength transfer from the repulsive to the attractive polaron is enhanced. Also, a weaker peak appears in the regime where the trion binding energy and the pairing gap are comparable, and provides a direct estimate of the interlayer exciton binding energy. Exciton density and spontaneous spin-valley polarization can also be easily read off from the polaron spectra. In conclusion, the polaron spectra carry the hallmarks of the excitonic insulator phase.

Can Xenes be excitonic insulators?

Friedhelm Bechstedt[1], Olivia Pulci[2], Paola Gori[3], Davide Grassano[4], Marco D'Alessandro[5]
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[5]ISM-CNR Rome, Italy

Xenes are two-dimensional (2D) honeycomb layers of group-IV elements carbon, silicon, germanium, tin, and lead. Recently, the Si-, Ge-, and Sn derived Xenes have been demonstrated to be topological as well as quantum spin Hall insulators. However their character under light illumination is under discussion.Trivial insulators are characterized by a fundamental gap E_g between conduction and valence bands, while an excitonic insulator (EI) fulfills the additional condition $E_b > E_g$ with E_b as the binding energy of the lowest exciton below the absorption edge. A topological insulator (TI) appears for band inversion, e.g. the exchange of s- and p-derived bands. It is mathematically defined by the topological invariant $Z_2=1$. A quantum spin Hall (QSH) insulator may show a quantized SH conductivity equal to the conductivity quantum e^2/h. Apart from measurements all these characteristic quantities can be investigated by means of modern electronic structure methods. Excellent examples for discussion of the four insulator types are freestanding Xenes silicene, germanene, stanene and plumbene, i.e. hexagonal graphene-like, but buckled 2D crystals of group-IV elements with honeycomb structure and resulting linear bands. Spin-orbit coupling (SOC) increasing along the group IV of the periodic table opens a fundamental gap and, therefore, produces heavy Dirac particles. In this talk important consequences of the linear Dirac band structure, the small SOC-induced gap E_g, the low screening on two-particle electron-hole excitations and a vertical electric field on band topology, exciton binding, and optical and spin Hall conductivities are discussed. The description of screening, not the band dispersion, rules the exciton binding and, consequently, the occurrence of the EI phase. Bulk-like screening as in quantum well structures tends to the stabilization of the EI phase while sheet screening mediated by the 2D electronic polarizability computed within DFT or model studies just like fully ab-initio many-body perturbation theory calculations suggest its absence. A vertical electric bias significantly varies the gap, the screening and finally defines a transition from the topological and QSH into a trivial insulator.

Exciton topology and condensation in a model quantum spin Hall insulator

Andrea Blason[1], Michele Fabrizio[1]

[1]International School for Advanced Studies of Trieste (SISSA), Italy

In this seminar, we explore the effects of local electron-electron repulsion on the single- and two-particle properties of a quantum spin Hall insulator, using a consistent mean-field approach. Specifically, we examine the Bernevig, Hughes, and Zhang model and find that the interaction between electrons leads to the emergence of an insulating and magnetoelectric phase that breaks inversion and time-reversal symmetries, but not their product. We observe that the softening of two exciton branches, each possessing finite and opposite Chern numbers, signals the approach to this phase from both topological and nontopological sides. Furthermore, we discuss the implications of these excitons, including their surface counterparts, on various physical observables. Overall, our study sheds light on the role of electron-electron repulsion in quantum spin Hall insulators and highlights the emergence of a novel phase that could be seen as a condensate of topological excitons.

Is Ta_2NiSe_5 a true excitonic insulator?

Girsh Blumberg[1], Mai Ye[1], Pavel Volkov[1], Amit Kanigel[2]

[1]Rutgers, the State University of New Jersey, USA
[2]Technion–Israel Institute of Technology, Israel

In a narrow-gap semiconductor, or a semimetal with slightly overlapping conduction and valence bands, excitons – electron-hole pairs bound together by Coulomb attraction – spontaneously form. Excitonic insulator is a coherent electronic phase that results from the formation of a macroscopic population of excitons. Excitonic insulators share similarities with the Bardeen-Cooper-Schrieffer superconductor: a distinctive broken symmetry, inherited by the exciton character, and collective modes of purely electronic origin. With only a few candidate materials known, the collective excitonic behavior is challenging to observe in solids, being obscured by crystalline lattice effects. Here we use polarization-resolved Raman spectroscopy to reveal the quadrupolar excitonic mode in the candidate zero-gap semiconductor Ta2NiSe5 disentangling it from the lattice phonons [1-3]. The excitonic mode pronouncedly softens close to the phase transition, showing its electronic character, while its coupling to noncritical lattice modes is shown to enhance the transition temperature.

The work was supported by the NSF-BSF under Grant No. DMR-2105001 and by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program Grant Agreement No. 885413.

1. Mai Ye *et al.*, PRB 104, 045102 (2021)
2. P. Volkov *et al.*, PRB 104, L241103 (2021)
3. P. Volkov *et al.*, npj Quantum Materials v. 6, 52 (2021)

Possible excitonic instability in AsCuLi2

Miki Bonacci[1], Davide Campi[2], Andrea Ferretti[1], Elisa Molinari[1,3], Nicola Marzari[4], Giovanni Pizzi[5], Deborah Prezzi[1], Marco Gibertini[1,3], Massimo Rontani[1], Daniele Varsano[1]

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[5]Paul Scherrer Institute, Switzerland

More than fifty years ago, hypotheses about the spontaneous Bose condensation of excitons in matter, i.e. without external optical excitation, were done [1]. This new theorized phase shows formal analogies with the superconductor ground state, albeit the nature of the order is different, and it may exhibit effects like macroscopic quantum coherence and exotic low-energy excitations. In this work we performed a high-throughput search for possible excitonic instability among thousands of recently discovered 2D monolayer materials, as obtained by computational exfoliation in 2018 [2] and contained in the Material Cloud 2D materials database (MC2D) [3]. We developed a dedicated screening protocol in order to discriminate candidates by applying state-of-the-art ab-initio methods, in particular many-body perturbation theory [4]. We accurately evaluated quasiparticle band structures and excitonic states via GW and BSE approaches, respectively. Robust computational workflows are implemented in the aiida-yambo plugin [5], a crucial tool needed in this work to perform the simulations in an automated high-throughput fashion. Preliminary but pushed convergence tests reveal that AsCuLi2, a topological insulator [6] isostructural to hexagonal Boron Nitride, may present spontaneous excitonic formation in its true ground state. Calculations are still ongoing, challenging the evaluation of excitonic states of AsCuLi2 within very high numerical accuracy (few meV, i.e. the accuracy of the method). A k dot p model Hamiltonian of the system has been developed consistently with the ab-initio findings, in order to describe the low-energy band structure in the neighborhood of the Gamma point and possibly derive a gap equation.

1. D. Sherrington and W. Kohn, Reviews of Modern Physics, 40(4):767-769, October (1968).
2. Mounet *et al*., Nature Nanotechnology, 13(3):246-252 (2018).
3. Mounet *et al*., Materials Cloud Archive, 2020.158(3) (2020).
4. Sangalli *et al*., J. Phys.: Condens. Matter, 31(32):325902 (2019).
5. Bonacci *et al*., arXiv:2301.06407 (2023).
6. Marrazzo *et al*., Nano Letters, 19(12):8431-8440 (2019).

Magnetic-field-induced Wigner crystallization of charged interlayer excitons in van der Waals heterostructures

Igor Bondarev[1], Yurii Lozovik[2]

[1]North Carolina Central University, USA
[2]Institute of Spectroscopy, RAS, Institute of Electronics and Mathematics, and Russian Quantum Center, Moscow, Russia

We develop the theory of the magnetic-field-induced Wigner crystallization effect for charged interlayer excitons (CIE) discovered recently in transition-metal-dichalcogenide (TMD) heterobilayers [1]. The Wigner crystal phase has been one of the longest anticipated exotic correlated phases, a phase that is very closely related to excitonic insulator, and originally was thought of as a periodic array of electrons held in place when their Coulomb repulsion energy exceeds the Fermi and thermal fluctuation energies. Here, we derive the ratio of the average potential interaction energy to the average kinetic energy for the many-particle CIE system subjected to the perpendicular magnetic field of an arbitrary strength, analyze the weak and strong field regimes, and discuss the ’cold’ crystallization phase transition for the CIE system in the strong field regime [2]. We also generalize the effective g-factor concept previously formulated for interlayer excitons [3], to include the formation of CIEs in electrostatically doped TMD heterobilayers. We show that magnetic-field-induced Wigner crystallization and melting of CIEs, the two correlated phases that block or allow the CIE transport in the system, can be observed in strong-field magneto-photoluminescence experiments with TMD heterobilayes of systematically varied electron-hole doping concentrations. Our results advance the capabilities of the TMD bilayers as a new family of transdimensional quantum materials.

1. L. A. Jauregui *et al.*, Science 366, 870 (2019).
2. I. V. Bondarev and Yu. E. Lozovik, Communications Physics 5, 315 (2022).
3. P. Nagler *et al.*, Nature Communications 8, 1551 (2017).

Anomalous plasmon dispersion in topological semimetals

Claudia Cardoso[1], Giacomo Sesti[1,2], Elisa Molinari[1,2], Daniele Varsano[1], Andrea Ferretti[1], Massimo Rontani[1]

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[2]FIM, University of Modena and Reggio Emilia, Italy

Monolayer WTe2 and MoTe2 are topological semimetals with similar crystal symmetry and band structure close to Fermi energy. However, at low temperature the former material becomes an excitonic insulator [1,2] and the latter a superconductor, possibly of the unconventional kind [3]. Intriguingly, a tiny amount of electron doping is sufficient to turn WTe2 into a superconductor as well [4]. This suggests that collective electronic excitations, which are responsible for the excitonic instability in WTe2, might play a major role throughout the whole doping range. Here we investigate plasmons in doped WTe2 and MoTe2 using both first principles and model approaches. Instead of the - standard - search of the roots of the longitudinal dielectric function within the random phase approximation, we solve the Bethe-Salpeter equation of motion for collective modes. This allows to resolve the multicomponent nature of the plasmon, since both intra- and inter-band electron-hole excitations contribute to the mode, as well as to capture the texture of the wave function in reciprocal space. As shown by our preliminary results for WTe2, the plasmon presents qualitative deviations from the behavior expected in 2d systems [5]: the plasmon dispersion dramatically flattens close to Brillouin zone center and quickly merges the electron-hole continuum as momentum increases, the low mode energy being weakly sensitive to doping.

This work is partially funded by MUR PRIN2017 No. 2017BZPKSZ “EXC-INS”.

1. Sun *et al.*, Evidence for equilibrium exciton condensation in monolayer WTe_2. Nature Phys. **18,** 94 (2022).
2. Jia *et al.*, Evidence for a monolayer excitonic insulator. Nature Phys. **18,** 87 (2022).
3. Rhodes *et al.*, Enhanced superconductivity in monolayer Td-MoTe2. Nano Lett. **21,** 2505 (2021).
4. Sajadi *et al.*, Gate-induced superconductivity in a monolayer topological insulator. Science **362,** 922 (2018).

Ground state symmetries and collective modes in Ta_2NiSe_5 - an excitonic insulator candidate

Banhi Chatterjee[1], Jernej Mravlje[1], Denis Golez[1]

[1]Jozef Stefan Institute, Slovenia

The origin of phase-transition from a high temperature orthorhombic phase to a low temperature monoclinic phase in Ta2NiSe5 is debatable. There are two competing scenarios, namely, a structural instability with a B2g zone center optical phonon and electronic order parameter of excitonic nature breaking the discrete set of lattice symmetries due to a spontaneous interband hybridization between Ta and Ni mediated by Coulomb many-body interactions [1-4]. We further explore the ground state symmetries and nature of collective excitations in the excitonic ordered phase of this compound. We perform a realistic modeling using Density Functional Theory as a starting point to construct a tight-binding Hamiltonian and describe the electronic correlations on a Hartree Fock level. The collective modes or excitonic susceptibilities in the ordered phase are computed within the linear response regime [5]. We see the breaking of discrete lattice symmetries due to the Ta-Ni hybridization makes the phase mode massive. The frequency of this phase mode scales with the strength of Ta-Ni hybridization. An amplitude mode appears at the gap edge and the intensity of it is less than the phase mode. The frequency of modes also shows a systematic dependence with temperature. We further discuss the need for inclusion of the electron phonon coupling to provide a complete picture of this phase transition.

1. A. Subedi, Phys. Rev. Mater. 4, 083601 (2020).
2. G. Mazza, M. Rösner, L. Windgätter, S. Latini, H. Hübener, A.J. Millis, A. Rubio, and A. Georges, Phys.Rev. Lett. 124, 197601 (2020).
3. L. Windgätter, M. Rösner, G. Mazza, H. Hübener, A. Georges, A. J. Millis, S. Latini, and A. Rubio,Angel, npj Comp. Mat 7, 1–14 (2021).
4. K. Katsumi *et. al*, arXiv: 2211.08537 (2022).
5. Y. Murakami, D. Golež, T. Kaneko, A. Koga, A.J. Millis, and P. Werner, Phys.Rev. B. 101, 195118 (2020).

Peculiar behavior in two-dimensional semimetals such as WTe_2

David Cobden[1]

[1]University of Washington, Seattle, USA

In two-dimensional materials that, according to band-structure calculations, should contain both electron and hole pockets, there is every reason to expect that electron-hole correlations will be strong and have significant consequences, such as formation of an excitonic insulator state. This is the situation in monolayer and bilayer WTe_2, which exhibit peculiar properties near charge neutrality. As these materials are cooled a thermodynamic gap opens up at the charge-neutral point, and the variation of the electrical conductivity with doping and temperature is impossible to reconcile with a single-particle band picture incorporating disorder. Calculations show that exciton binding here should very strong, and it is natural to ask whether formation and condensation of equilibrium excitons can explain the observed behavior. While the opening of a gap appears consistent with formation of an excitonic insulator, understanding the conductivity when the electron and hole densities are unbalanced is beyond the excitonic insulator model and calls for new experimental approaches as well as theoretical insights. We are attacking this question by modifying the WTe_2 and by searching for other two-dimensional semimetals exhibiting similar behavior.

Chester supersolid of excitons in semiconductor heterostructures

Sara Conti[1], Andrea Perali[2], Alex Hamilton[3], Francois Peeters[4], Milorad Milosevic[1], David Neilson[1]

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[2]Supernano Laboratory, University of Camerino, Camerino, Italy
[3]University of New South Wales, Sydney, Australia
[4]Universitade Federal do Ceara, Fortaleza, Brazil

A supersolid, a counter-intuitive quantum state in which a rigid lattice of particles flows without resistance, has to date not been unambiguously realized. Here we reveal a supersolid ground state of excitons, formed from spatially separated electrons and holes in a semiconductor heterostructure. The supersolid is driven by a large exciton dipole moment and occurs at electron-hole separations lying outside the focus of recent transport experiments on exciton superfluidity in double layer systems [1]. Our supersolid conforms to the original Chester concept of a supersolid [2] with one exciton per supersolid site. It is distinct from an alternative version observed in cold-atom systems which is characterized by a cluster of condensates [3]. In the phase diagram, the new supersolid phase appears at electron-hole separations much smaller than for the predicted exciton normal solid [4], and it persists up to a solid-solid transition where the quantum phase coherence collapses while leaving the translational symmetry preserved. The ranges of electron-hole separations and exciton densities in our phase diagram are well within reach of current experimental capabilities.

1. Z. Wang *et al.*, Nature 574, 76 (2019); L. Ma *et al.*, Nature 598, 585(2021).
2. G. V. Chester, Phys. Rev. A 2 256 (1970).
3. M. A. Norcia *et al.*, Nature 596, 375 (2021).
4 G. E. Astrakharchik, J. Boronat, I. L. Kurbakov, and Yu. E. Lozovik, Phys. Rev. Lett. 98, 060405 (2007).

Excitons in bilayer WTe_2

Matteo D'Alessio[1,2], Elisa Molinari[1,2], Daniele Varsano[2], Massimo Rontani[2]

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[2]CNR-NANO, Modena, Italy

Bilayer WTe2 is a remarkable two-dimensional metal, since it exhibits a macroscopic out-of-plane electric dipole in spite of the presence of charge carriers that screen the electrostatic forces between ions [1]. Intriguingly, at low temperature the system develops a narrow transport gap, which has many-body origin and was attributed to the permanent condensation of excitons, electron-hole pairs bound by Coulomb attraction [2]. Contrary to other known bilayer excitonic insulators, in which electrons and holes are spatially separated, in WTe_2 interlayer tunneling is significant. This might impact the observable features of the putative exciton condensate, giving rise to a coherent contribution to the electric dipole, due to the interband electric polarization of excitons. In this work we investigate bilayer WTe2 from first principles, focusing on excitons by solving the Bethe-Salpeter equation of motion. The ultimate goal is to assess the instability of the system against exciton condensation, as well as to predict its possible experimental fingerprint.

1. Fei *et al*., Ferroelectric switching of a two-dimensional metal. Nature **560,** 336-339 (2018).
2. Sun *et al*., Evidence for equilibrium exciton condensation in monolayer WTe_2. Nature Physics, **18,** 94–99, (2022).

Correlated phases in AB-stacked twisted TMD bilayers

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Twisted bilayers of transition metal dichalcogenides (TMD) have emerged as a novel platform for the realisation of strongly correlated phases of matter. Among other reasons, there is a great interest in TMDs because they are good candidates to host the so long sought excitonic insulating phase, that is stabilized by condensation of excitons, i.e. bound pairs of electrons and holes. The forbidden hybridization between two different AB stacked homobilayers could facilitate the condensation of inter-layer excitons, that could explain the insulating phases observed in twisted homobilayers of WSe_2. Also a Curie-Weiss 1/T behavior of the magnetic susceptibility has been reported for this material pointing to the formation of local moments, a hallmark of strong correlations. However, the precise nature of such an insulating phase has not yet been determined for the excitonic order could coexist with a charge-transfer insulator, Mott insulator or it could lead to a supersolid phase. Here we present a study of the SU(4) Heisenberg and Hubbard models in the triangular lattice, that should capture the salient features of AB-stacked TMD homo-bilayers, using different many-body theoretical techniques, such as spin-wave theory and Dynamical Mean Field Theory (DMFT).We show how the system in presence of a finite layer imbalance, that is experimentally obtained using a bias voltage between the two layers, naturally hosts multi-Q order states which are inter-layer excitonic insulators with a spin texture which modulation (i.e. Q-vector) is layer resolved. Furthemore, the order phase passes from commensurate to incommensurate at a critical value of the inter-layer polarisation which marks a quantum criticality. We studied also the metal-to-insulator transition occuring in the SU(4) Hubbard model in a broken symmetric phase which is determined by the three M points in the Brillouin zone, and we sketched a phase diagram as a function of the Coulomb repulsion and filling.

From Mott insulators to checkerboard solids with dipolar excitons

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Dipolar excitons of bilayer heterostructures provide unique opportunities to experimentally explore collective phases accessible to strongly correlated bosonic systems. In fact, by enforcing a spatial separation between electrons and holes constituting dipolar excitons, one imprints a permanent gigantic electric dipole, yielding strong quasi-long-range dipolar repulsions between excitons. Here, we report studies emphasising dipolar excitons of GaAs bilayers. We manipulate the interaction between the excitons dipole and a gate defined electric field to confine dipolar excitons in 200 to 500 nm period lattice potentials. Then, we evidence that on-site repulsive dipolar interactions stabilise Mott insulating phases at sub-Kevin temperatures, with either one or two excitons uniformly filling up to 100 lattice sites. For sufficiently small lattice periods, we further show that dipolar excitons allow for the first implementation of the Bose-Hubbard model extended by nearest neighbour interactions, so that an insulating phase is stabilised at half-filling, excitons thus realising a checkerboard density wave.

Order, criticality, and excitations in the extended Falicov-Kimball model: A case study for the strong excitonic insulator candidate Ta_2NiSe_5

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We investigate the nature of excitonic bound states and the emergence of exciton coherence in the one-dimensional half-filled extended Falicov-Kimball model (EFKM) by means of unbiased numerical techniques. The EFKM ground-state phase diagram exhibits, besides band-insulator and staggered orbital ordered phases, an excitonic insulator (EI) state with power-law correlations. The criticality of the EI state shows up in the von Neumann entropy. The anomalous spectral function and condensation amplitude provide the binding energy and coherence length of the electron-hole pairs which, on their part, point towards a Coulomb interaction driven crossover from BCS-like electron-hole pairing fluctuations to tightly bound excitons. In a non-equilibrium situation, we demonstrate photoinduced pairing of electron and holes as well as metallization of the EI. In the latter case, an extra band appears above the Fermi energy after pulse irradiation, indicating an insulator-to-metal quantum phase transition. For model parameters best suited for Ta_2NiSe_5 the photoemission spectrum develops a weak but clearly visible two-peak structure around the Fermi momenta $k \simeq \pm k_F$, suggesting that Ta_2NiSe_5 embodies an EI of BCS-like type. At higher temperatures, the leakage of the conduction-electron band beyond the Fermi energy becomes distinct, which might serve as an explanation for the bare non-interacting band structure seen in time- and angle-resolved photoemission spectroscopy experiments.

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Origin of spatial modulations of the local density of states in WTe_2

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WTe_2 is a transition metal dichalcogenide (TMD) that crystallizes in the 1T' structure - a distortion of the 1T phase creating 1D zig-zag chains of metal atoms. First-principles calculations predict a semimetallic bulk [1] and spectroscopic measurements of monolayer WTe_2 grown on conductors report an insulator with average bandgap in the range 10-100 meV [2,3], while electronic transport measurements of WTe_2 grown on insulators reveal an insulating bulk with dissipationless edge states that persist up to 100 K [1,3]. New evidence [4,5] suggests the bandgap is not only topological, but excitonic in origin, implying WTe_2 is an interaction-driven insulator. To shed light on the nature of WTe_2 bandgap, we carried out scanning tunnelling microscopy and spectroscopy experiments at ultra-low temperatures (1.2K) and in the presence of a magnetic field up to 3 T. We discuss the spatial modulation of the local density of states as observed via scanning tunneling spectroscopy [2,6] in terms of formation of electron-hole pairs and charge density waves [2] or quasi-particle interference [6].

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Symmetries and collective mode in excitonic insulators

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In excitonic insulator candidates, like 1T-$TiSe_2$ and Ta_2NiSe_5, the simultaneous presence of structural distortions and strong Coulomb interaction prevents a transparent classification of the driving mechanism for the symmetry-breaking transition. I will present how collective response can be employed to classify the importance of each degree of freedom and gauge them with experimental data. I will focus on the collective mode dynamics in realistic models of Ta_2NiSe_5, which leads to much richer physics than typically anticipated from minimal models. The modelling explains how the amplitude and the phase modes are realized in the material and what are its symmetry properties. Considering the realistic band structure, I will show that the mass of the phase mode can reveal how the electronic symmetry is reduced in the material. Remarkably, the collective mode analysis shows that previously reported phases are not in the ground state unless the system exhibits strong coupling with lattice degrees of freedom. These symmetry arguments give firm boundaries on the competition between microscopic degrees of freedom and we propose non-linear optical processes which are directly sensitive to the collective response. The study will explain how a combination of realistic modelling and symmetry arguments is a generic tool for understanding the rich collective mode structure, and it should be employed in other excitonic insulator candidates.

Transport signature of magnetoexciton insulating state in electron-hole graphene double-layers

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Charged carriers in partially filled Landau levels in a double layer quantum well can bind to form magnetic excitons across the insulating layer. For complementary filled electron-hole Landau levels in the double layers, insulator magnetoexciton condensation can be produced, demonstrating superfluidic exciton flows without a quantum Hall edge state. We report the observation of the electron-hole bound magnetoexciton insulator state in two layers of graphene separated by a few nanometers of hexa-boron nitride under strong magnetic fields. We observe that the conduction in the first graphene layer vanishes when the second graphene layer is open-circuited. However, when the circuit of the second layer is closed, the first layer becomes conductive and a perfect drag current is induced in the second layer. In the counter-current geometry, we observe vanishing longitudinal and Hall resistances, which is indicative of the superfluidic transport of the charge-neutral magnetoexciton condensate. Using gate voltage and magnetic field, we study the condensate phase diagram as a function of temperature and magnetic field, which control the exciton density.

Quantum Hall superfluid in twisted bilayer/double bilayer graphene

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We introduce a novel two-dimensional electronic system with ultrastrong interlayer interactions, namely twisted bilayer graphene with a large twist angle, as an ideal ground for realizing interlayer-coherent excitonic condensates. In these systems, subnanometer atomic separation between the layers allows significant interlayer interactions, while interlayer electron tunneling is geometrically suppressed due to the large twist angle. By fully exploiting these two features we demonstrate that a sequence of odd-integer quantum Hall states with interlayer coherence appears at the second Landau level (N = 1). Notably the energy gaps for these states are of order 1 K, which is several orders of magnitude greater than those in GaAs. Furthermore, a variety of quantum Hall phase transitions are observed experimentally. All the experimental observations are largely consistent with our phenomenological model calculations. Hence, we establish that a large twist angle system is an excellent platform for high-temperature excitonic condensation.

We also observed similar states in a stack of two decoupled graphene bilayers. Indeed, such a Bose-Einstein condensate is observed for half filling in each bilayer sheet when the partially filled level has orbital index 1, whereas it is absent for partially filled levels with orbital index 0. The application of asymmetric top and bottom gate voltages enables to influence the orbital nature of the electronic states of the graphene bilayers and to navigate in an orbital mixed space. The latter hosts an even denominator fractional quantum Hall state at total filling -3/2. Our observations suggest a unique edge construction involving both electrons and chiral p-wave composite fermions.

Materials design of magnetic and topological excitonic insulators from first-principles

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Magnetic/topological excitonic insulators combine magnetism/nontrivial-topology and spontaneous exciton condensation, with dual functionality of magnetic/topological insulators and excitonic insulators. Yet, they are very rare and little is known about their formation. In this presentation I will describe our recent progress in finding and designing two-dimensional magnetic excitonic insulators and topological excitonic insulators using first-principles GW-BSE calculations in accordance with the selection rule. We reveal an unusual electronic state (dubbed as half excitonic insulator) in monolayer 1T-MX_2 (M = Co, Ni and X = Cl, Br). Its one spin channel has a many-body ground state due to excitonic instability, while the other is characterized by a conventional band insulator gap. We predict the semi-hydrogenated graphene (known as graphone) as a spin-triplet excitonic insulator with a critical temperature of 11.5 K. We find that a mechanism dubbed as parity frustration prevents excitonic instability in usual topological insulators, and those whose band inversion is independent of spin-orbit coupling are possible candidates. We verify this on four monolayer double-transition-metal carbides (MXenes), which show a robust thermal-equilibrium exciton condensation, being sufficient for topological applications at room temperature.

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Non reciprocal phase transitions in polaritonic systems

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We propose a novel mechanism for a nonequilibrium phase transition in a U (1)-broken phase of an electron-hole-photon system, from a Bose-Einstein condensate of polaritons to a photon laser, induced by the non-Hermitian nature of the condensate. We show that a (uniform) steady state of the condensate can always be classified into two types, namely, arising either from lower or upper-branch polaritons. We prove (for a general model) and demonstrate (for a particular model of polaritons) that an exceptional point where the two types coalesce marks the end point of a first-order-like phase boundary between the two types, similar to a critical point in a liquid-gas phase transition. We discuss how this generalises into non-reciprocal classical systems.

Hidden excitonic quantum states with broken time reversal symmetry

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The physical manifestations of the state of matter known as excitonic insulator strongly depend on the degrees of freedom it couples with. For instance, the excitonic instability in a crystalline system may result in a distortion of the charge density whose coupling with the ionic degrees of freedom can mask the nature of the excitonic insulator. In this seminar, I will discuss how a dichotomic manifestation of the symmetry breaking underlying an excitonic phase transition can be engineered to stabilise a purely orbital time-reversal symmetry broken (TRSB) hidden quantum state in a two-dimensional (2D) material. I will show the formation of the TRSB state driven by a self-generated flux which sustains equilibrium orbital currents issuing from the excitonic instability. The transition to the TRSB excitonic state is controlled by means of engineered geometrical constraints which, in a cylindrical geometry, enable coupling between the excitonic order parameter and free space electromagnetic field. I will discuss implication of these results for the stabilization of exotic TRSB states in quantum materials and the disentangling of coupled excitonic and structural transitions.

Ab initio predictions of new exciton insulators

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Van der Waal heterostructures provide promising platforms to study exciton condensation since they can host long lived excitons formed by spatially separated electron-hole pairs. In double bilayer graphene experimental evidence of exciton condensation was found 2018 (W. Burg et al. Phys. Rev. Lett. 120, 2018). Recently also MoSe2/WSe2 bilayers have been shown to become excitonic insulators at certain electron and hole concentrations (Wang et al., Nature 574, 2019; L. Ma et al., Nature 598, 2021). In all these experimental setups the electron hole layers were separated by dielectric barriers and the electron and hole concentrations were tuned using external gates. In this work we explore how novel exciton insulators and exciton superfluids can be formed in bilayers of TMDs and Janus materials, without the need for external gates and insulating barriers. Our work combines state-of-the-art tools, such as the GW-approximation, Quantum Electrostatic Heterostructure model (Andersen et al. Nano Lett. 15, 2015) and Exciton Density Functional Theory (Nilsson et al. Phys. Rev. Mat. 5, 2021) with a new downfolding procedure that allows for ab initio modelling of exciton superfluidity in general van der Waal heterostructures (Nilsson et al. J. Phys. Chem. Lett. 14, 2023).

Bulk MoS2 under pressure as an excitonic insulator

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The investigation of the mechanisms driving the stabilization of charge density waves (CDW) in low-dimensional crystals has garnered a great deal of attention from the ab initio community in recent years. In this contribution, we discuss the case of bulk MoS_2 at low temperature (< 10 K) and ultra-high hydrostatic pressure (~ 20-30 GPa) and argue that here a CDW transition can be explained as purely induced by the nonlocal part of the electron-electron interaction: i.e., this system is a candidate for being a real excitonic insulator. Firstly, we show that at the critical pressure, an exciton with finite center-of-mass momentum acquires negative energy in the absence of a corresponding softening of phonon modes. This leads to a purely electronic phase transition with the appearance of a CDW with antiferroelectric character. Secondly, we theoretically investigate the inelastic X-ray scattering spectra of bulk MoS_2 under pressure. We discuss the pressure dependence of the rich fine structure appearing in the resulting spectra including both lattice vibrations and neutral electronic excitations, in order to track the possible pathways of both excitonic and phononic instabilities towards the CDW phase transition.

Josephson effect and superfluidity in exciton heterobilayers

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We analyze the superfluid characteristics and crossover physics for different Josephson junctions [1] in exciton heterobilayers TMD semiconductors [2]. The type II interface has been demonstrated to host a strongly correlated excitonic insulator [3]. We determine the Josephson critical current for different potential barrier heights [4,5]. We show that the crossover physics in the narrow barrier region controls the critical current throughout. We find that the ratio of the critical current divided by the carrier density exhibits an observable maximum at the density of the switchover from bosonic excitations to pair-breaking fermionic excitations. This provides, for the first time in a semiconductor system, an experimental measure for the position of the boundary separating the BEC and BCS-BEC crossover regimes.

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Theory of disordered excitonic insulators

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An excitonic insulator (EI) is an unconventional quantum phase of matter in which excitons, bound pairs of electrons and holes, undergo Bose-Einstein condensation. While several materials have emerged as promising EI candidates, distinguishing a possible EI from a normal insulator remains challenging. To address this, we focus on a clear qualitative difference between these two phases: the spontaneous breaking of a unique excitonic U(1) symmetry gives rise to low-lying Goldstone collective modes in the EI gap. We consider how disorder affects these collective modes. We show that different disorder symmetries lead to qualitatively different collective mode scattering rates. Notably, we find that unlike electrons, collective modes are highly robust against disorder that respects excitonic U(1) symmetry, implying a unique experimental fingerprint: the ballistic propagation of low-lying modes over mesoscopic distances, at electronic-scale velocities. We suggest this feature could affect thermal transport at low temperatures, and might be observed in spatially resolved pump-probe spectroscopy as Goldstone-phonon hybridized modes. In novel two-dimensional EI platforms, our treatment of EI disorder screening may be applicable to the polaron impurity problem and the modelling of device inhomogeneity.

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Excitonic vs Mott insulator in carbon nanotubes: A proposed experimental test

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Ultraclean, nominally metallic carbon nanotubes upon suspension always display a residual, intrinsic gap at the charge neutrality point. This gap is thought to have a many-body origin, associated with either a Mott [1] or an excitonic phase [2,3]. The two scenarios are fundamentally different, as a Mott phase [1] is driven by the short-range part of the Coulomb interaction, while an excitonic phase [2] is originated by the long-range part of the Coulomb interaction. Despite the two phases being characterised by different symmetry properties, an exhaustive experiment is still lacking. Here we show that the distinctive feature of the excitonic insulator phase is the presence of a cusp in the dispersion of the gap with the axial magnetic field, close to the gap minimum. On the contrary, the Mott phase exhibits a featureless, rounded profile. The non-analytic spike originates from the extreme sensitivity of electon-electron interactions to the Aharonov-Bohm gap modulation. This is demonstrated on the basis of a model for screening [4] developed by us adapt for tubes of different size and chirality, capable to replicate first-principle computations of the electron-electron interaction in nanotubes.

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Excitonic insulator phase in narrow-gap carbon nanotubes

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Pristine single-wall carbon nanotubes are an exciting class of systems, showing a variety of interaction-driven phenomena [1,2]. Many-body effects are also thought to be responsible for the residual gap observed in the subset of nanotubes that band theory predicts to be metallic when undoped. The correlated phase generated in these tubes has a disputed origin: a Peierls instability [3], a Mott Insulator [4] or an excitonic insulator [5]. Here, we follow the idea of carbon nanotubes as excitonic insulators. By making use of a model of screening [6] adapt for tubes of different size and chirality, validated from state-of-art first-principle computations, we determine the excitonic energies on a large set of narrow-gap tubes. Eventually, we find that all the tubes considered are potentially subject to an excitonic instability at low temperatures. We then compute the phase diagram associated to the reconstructed excitonic ground state as a function of tubes chirality and radii.

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Electrical breakdown of excitonic insulators

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We propose a new electrical breakdown mechanism for exciton insulators in the BCS limit, which differs fundamentally from the Zener breakdown mechanism observed in traditional band insulators. Our new mechanism results from the instability of the many-body ground state for exciton condensation, caused by the strong competition between the polarization and condensation energies in the presence of an electric field. We refer to this mechanism as "many-body breakdown". To investigate this new mechanism, we propose a BCS-type trial wave function under finite electric fields and use it to study the many-body breakdown numerically. Our results reveal two different types of electric breakdown behavior. If the system size is larger than a critical value, the Zener tunneling process is first turned on when an electrical field is applied, but the excitonic gap remains until the field strength reaches the critical value of the many-body breakdown, after which the excitonic gap disappears and the system becomes a highly conductive metallic state. However, if the system size is much smaller than the critical value, the intermediate tunneling phase disappears since the many-body breakdown happens before the onset of Zener tunneling. The sudden disappearance of the local gap leads to an "off-on" feature in the current-voltage curve, providing a straightforward way to distinguish excitonic insulators from normal insulators.

Excitonic insulator in a Bilayer WSe2/monolayer WS2 moiré superlattice

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Two-dimensional moiré superlattices provide a highly tunable platform to study strongly correlated physics. In particular, the moiré superlattices of two-dimensional semiconductor heterojunctions have been shown to host tunable correlated electronic states such as a Mott insulator and generalized Wigner crystals. Here we report the observation of an excitonic insulator, a correlated state with strongly bound electrons and holes, in an angle-aligned monolayer WS2/bilayer WSe2 moiré superlattice. The moiré coupling induces a flat miniband on the valence-band side only in the first WSe2 layer interfacing WS2. The electrostatically introduced holes first fill this miniband and form a Mott insulator when the carrier density corresponds to one hole per moiré supercell. By applying a vertical electric field, we tune the valence band in the second WSe2 layer to overlap with the moiré miniband in the first WSe2 layer, realizing the coexistence of electrons and holes at equilibrium, which are bound as excitons due to a strong Coulomb interaction. We show that this new bound state is an excitonic insulator with a transition temperature as high as 90 K. Our study demonstrates a moiré system for the study of correlated many-body physics in two dimensions.

Optical detection of excitonic insulators in van der Waals heterobilayers: Progress and future prospects

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Semiconductors and semimetals with strong Coulomb interactions are expected to exhibit a state of matter known as excitonic insulators (EXI), where the ground state at T=0 K is a Bose-Einstein condensate (BEC) of excitons [1]. This BEC of excitons forms when the bandgap between the conduction band minimum and valence band maximum is smaller than the binding energy of an electron-hole pair, resulting in an insulating state of matter with EXI characteristics. This ground state has potential applications in investigating strongly correlated bosons and creating an interacting degenerate Bose-Fermi mixture of excitons and itinerant electrons. This study aims to investigate the possibility of realizing EXI through the condensation of interlayer excitons. To achieve this, a heterobilayer device has been selected with MoS_2 and WSe_2 transition metal dichalcogenides due to their Type-II band alignment. The device consists of a thin hexagonal boron nitride (hBN) dielectric layer that can withstand high electric fields and facilitate the closing of the interlayer band gap via electrostatic gating. This study employs Bose polaron spectroscopy to investigate the excitonic insulator state and detect the emergence of attractive and repulsive polarons that result from intralayer excitons dressed by ground-state interlayer excitons. Previous work by I. Amelio et al. [2] has suggested that the differences in the spectra of Bose and Fermi polarons could offer a new approach to identifying the presence of ground-state interlayer excitons. In addition, a recent study on Bose polarons in cold atoms [3] has shown a significant energy shift of the polaron resonance at the onset of the critical temperature for condensation, indicating that temperature-dependent Bose polaron spectroscopy may provide insight into the signature of EXI in van der Waals heterostructures.

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Theory of the excitonic insulator phase in monolayer WTe2

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Fresh evidence [1,2] suggests that monolayer WTe_2 is the long-sought excitonic insulator (EI), a permanent Bose-Einstein condensate of excitons that form in the absence of optical excitation. A surge of experimental claims has recently addressed layered materials, because of reduced Coulomb screening. However, the transition to the putative EI is ubiquitously accompanied by the softening of a phonon inducing a structural change; therefore, it remains unclear whether the observed phase is genuinely excitonic or instead stabilized by electron–phonon interaction. On the contrary, no charge density wave is seen in WTe_2, which rules out the role of lattice distortion in this material. Here we present a full theory of the EI phase of WTe_2, which is consistent with the key experimental findings at charge neutrality and builds on unbiased calculations from first principles. The ab initio solution of the Bethe-Salpeter equation shows that the exciton binding energy is larger than 100 meV and the radius as small as 4 nm, explaining the observed formation of excitons at high temperature and doping levels [1]. The excitons responsible for the instability experience giant exchange interactions (of the order of 20 meV), which originate from the strong spin-orbit coupling that hybridizes conduction and valence bands. As a consequence, the EI ground state is a spin density wave. The multivalley mean-field calculation of the EI chemical potential as a function of doping is in quantitative agreement with the experiement. Finally, we predict unique features of the EI phase to appear in photoemission and THz absorption spectra.
This work is partially funded by MUR PRIN2017 No. 2017BZPKSZ “EXC-INS”.

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Spin-triplet topological excitonic insulators in two-dimensional materials

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Quantum spin-hall insulator (QSHI) processes nontrivial topology. We notice that the electronic structures of some particular QSHIs are favorable for realization of excitonic insulators (EIs). Using first-principles many-body perturbation theory (GW+BSE) and k dot p model, we show that high-temperature (T) topological EIs with unlike spin can exist in such QSHIs with non-vanishing band gaps, e.g. 2D AsO and $Mo_2TiC_2O_2$. Spin-triplet type EI phase induced by strong electron-hole interaction preserves time-reversal symmetry and the topological characteristics. A novel optical selection rule exists, upon going through the phase transition from the normal QSHIs to the topological EIs, absorption spectroscopy shows pronounced T-dependent changes, providing guidance for future experimental detections. The demonstrated coupling between EIs and topology also means that rich physics exists in such materials which retain such interdisciplinary features.