Moire Physics in Semiconductors

Liang Fu

2023 Theory Winter School at MagLab

Two-dimensional atomic crystals (2005)

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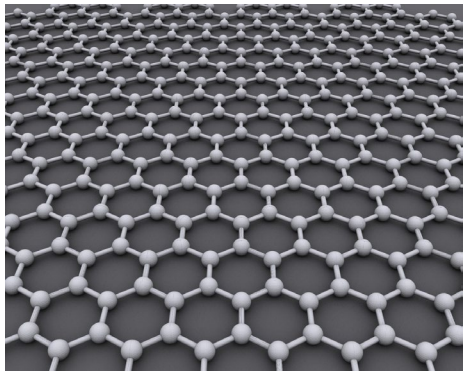
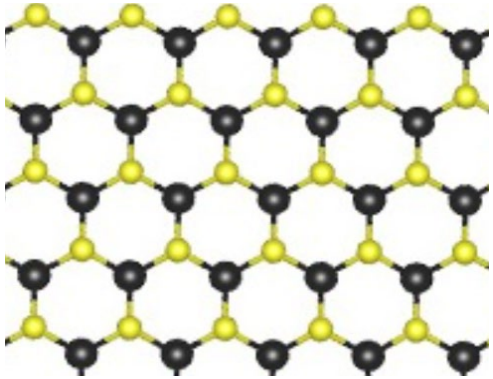
Graphene



Transition metal dichalcogenides
MX_2



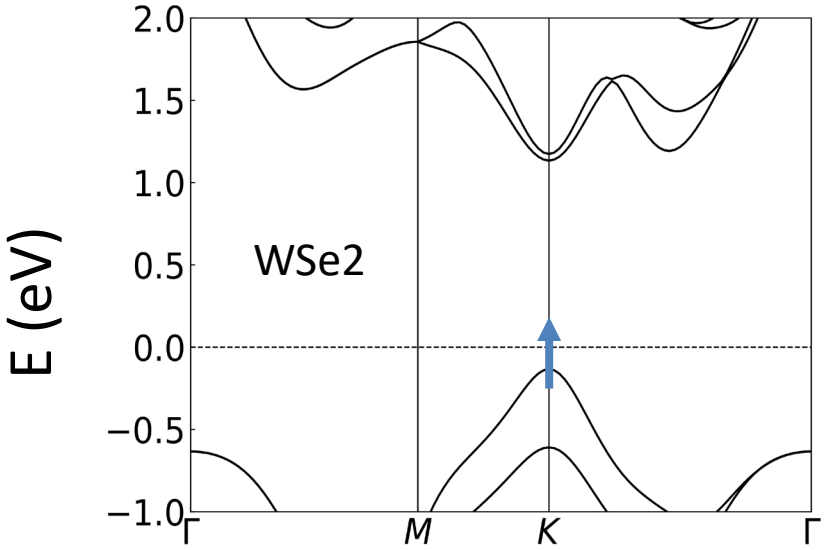
Big Family of 2D TMDs

MX_2 : M = W, Mo, Nb, Ta
X = Te, Se, S

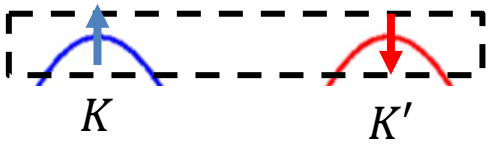
- **semiconductors**: WSe_2
- superconductors: $NbSe_2$
- charge density waves: TaS_2
- topological insulators: WTe_2

Monolayer Semiconductor MX_2

M=W, Mo and X=Te, Se, S

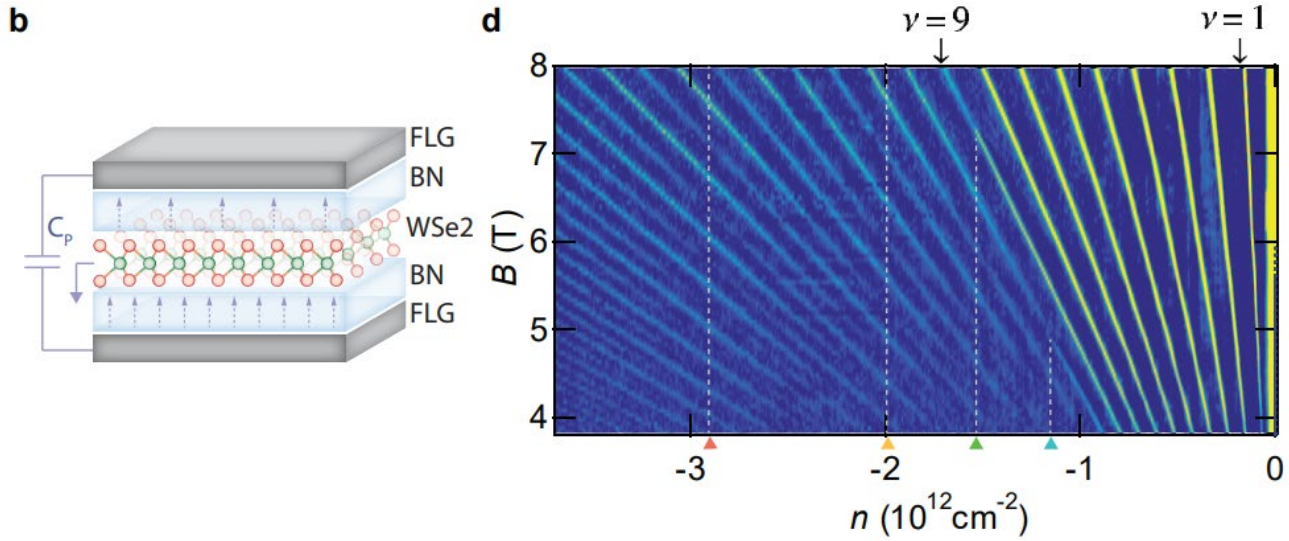


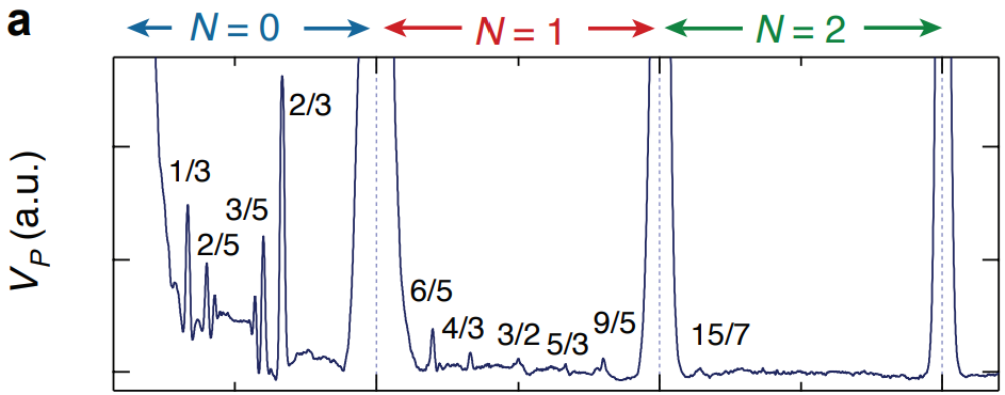
$$H = \sum_i \frac{p_i^2}{2m} + \frac{1}{2}\sum_{i\neq j} \frac{e^2}{\epsilon|r_i - r_j|}$$



- parabolic valence/conduction band
- spin-valley locking in $\pm K$ valleys
- large effective mass $\sim 0.5 - 1 m_e$ (cf. TBG)

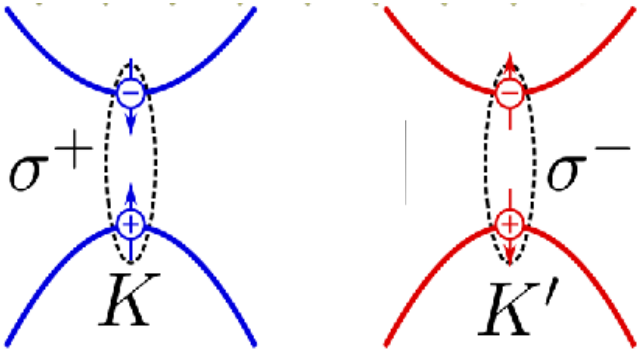
2DEG in Monolayer TMD

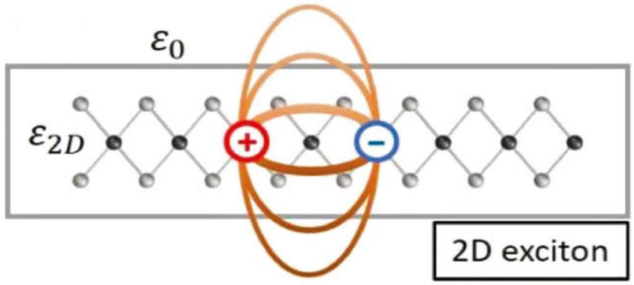


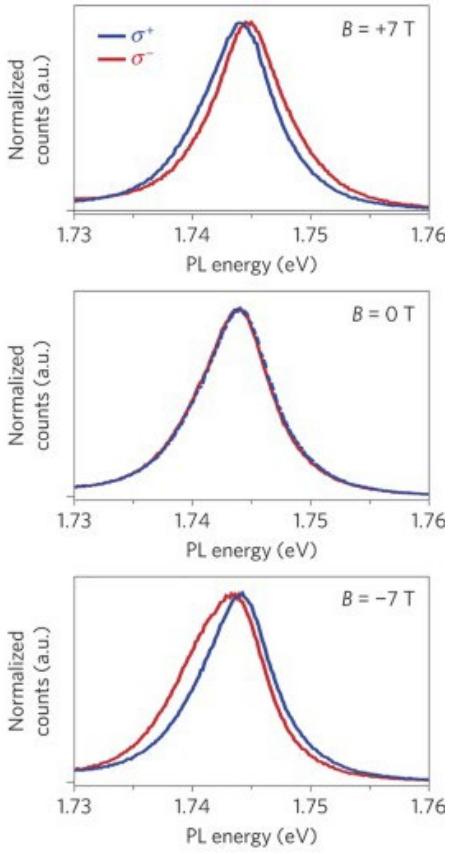


Shi et al, Nat. Nano. (2020)

Optical Response & Exciton Physics





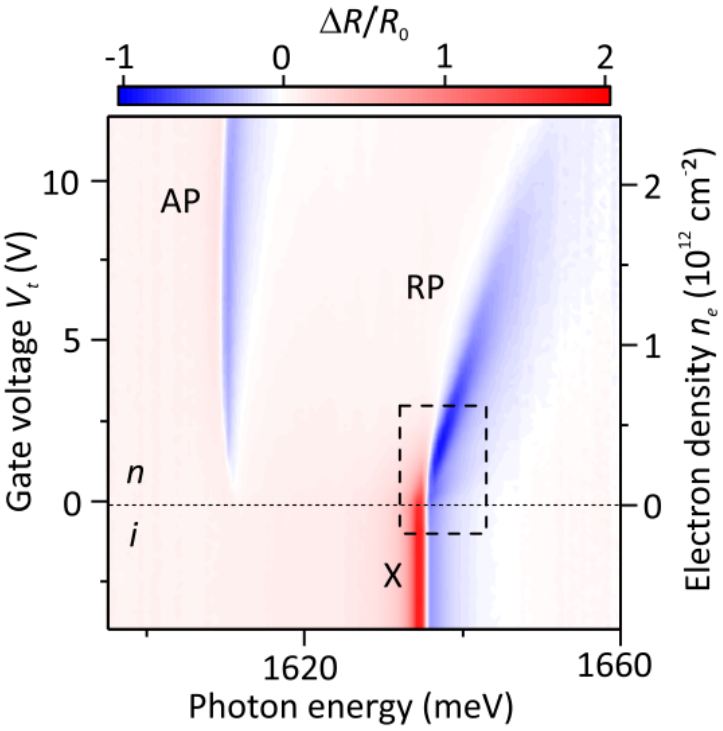


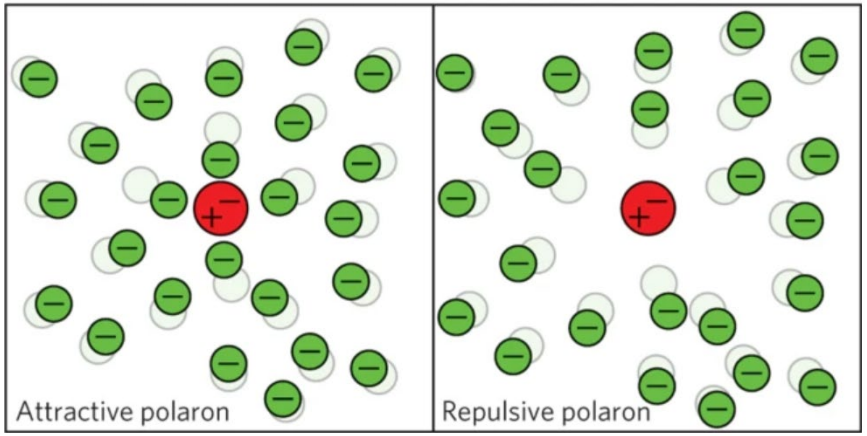
Aivazian et al, Nat. Phys (2014)

- exciton: large binding energy; small Bohr radius
- valley selection rule and Zeeman splitting

Exciton in Electron Liquid

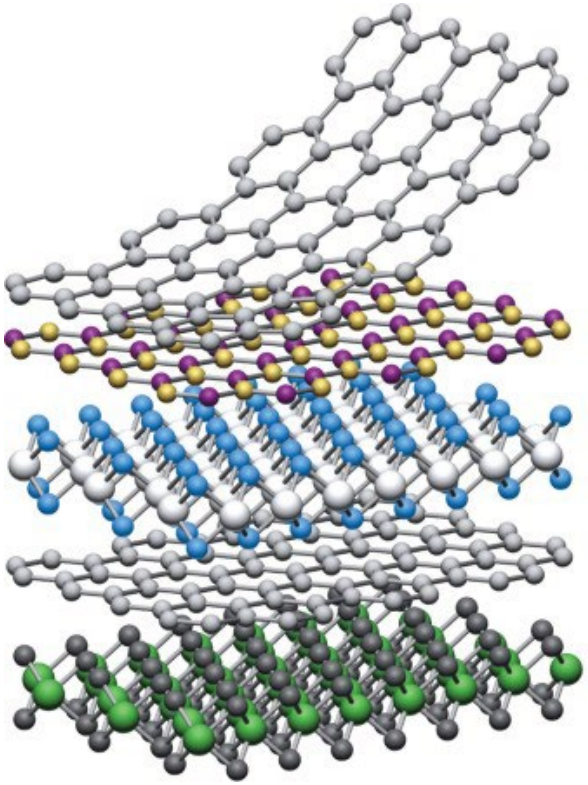
Monolayer $MoSe_2$ at B=0

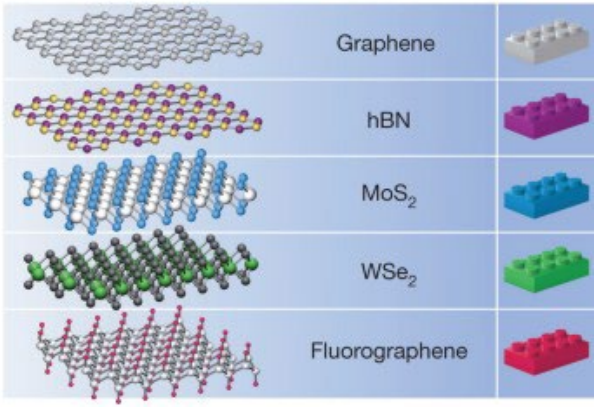


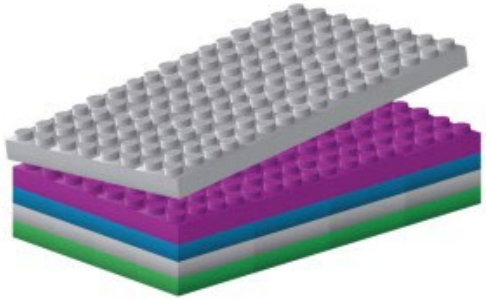


Smolenski et al, Nature (2020)

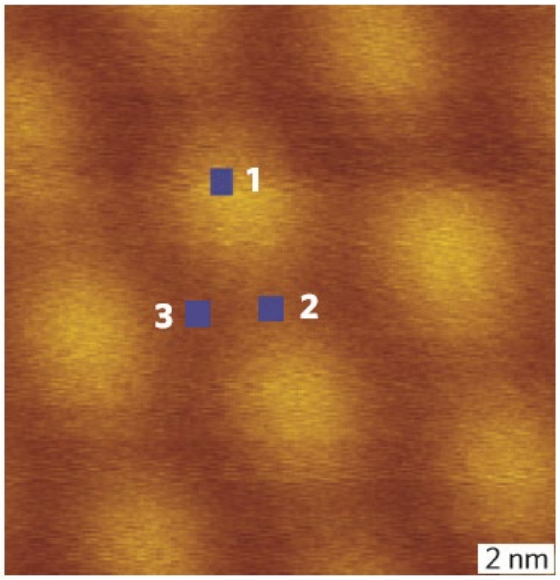
VdW Heterostructures: 1+1>>2



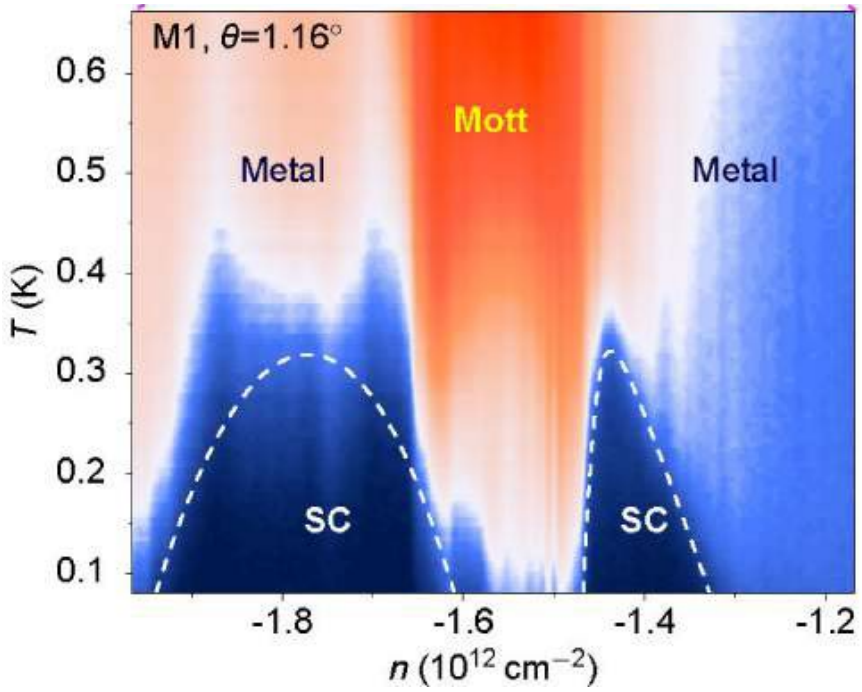




Moire Superlattices



Li et al, Nat. Phys (2010)

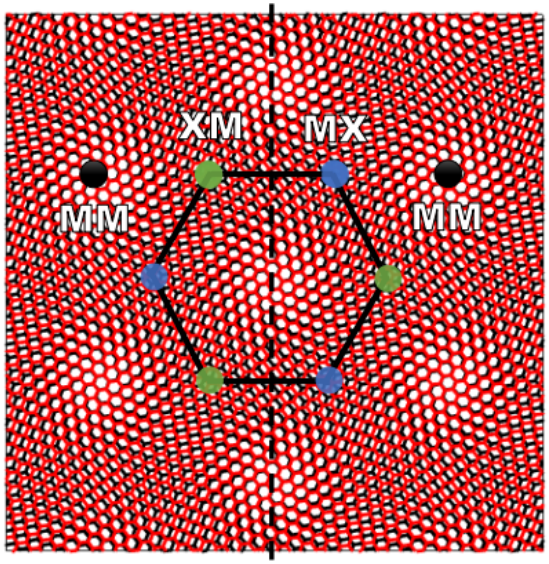


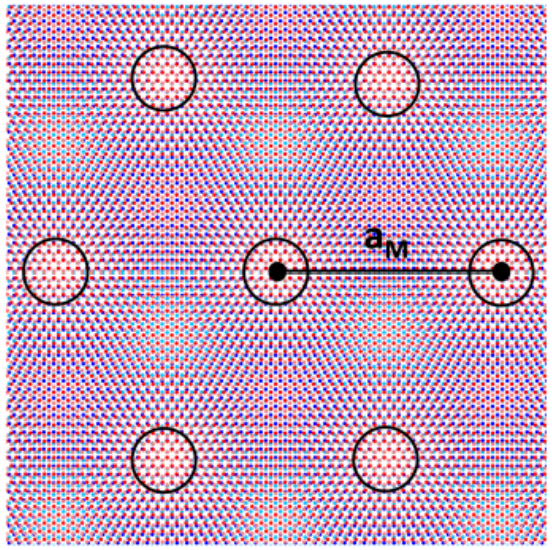
Cao et al, Nature (2018)

Semiconductor Moire Superlattices

twisted homobilayer

heterobilayer
(twist not needed)



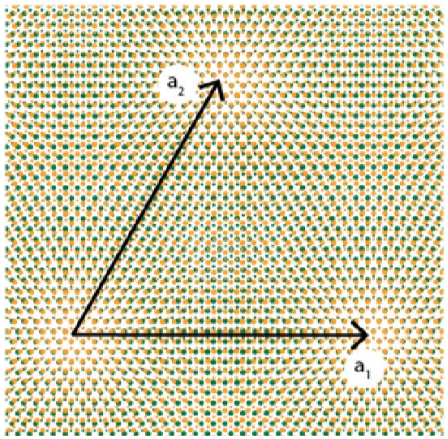


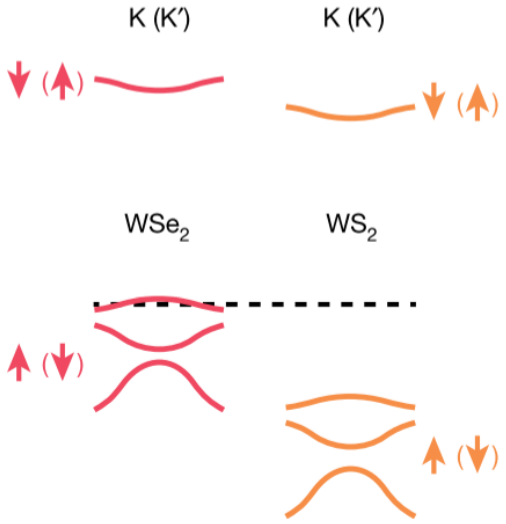
Moire period depends on lattice mismatch and twist angle:

$$a_M = \frac{a}{\sqrt{\theta^2+\delta^2}}, \quad \delta = 1 - \frac{a'}{a}$$

Moire Band in Heterobilayer

WSe_2/WS_2





Spatial variation of band edge due to <u>lattice corrugation</u> generates slowly-varying periodic potential

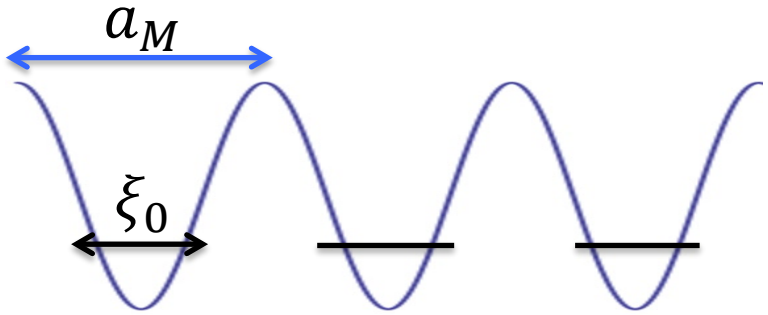
$$H = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{r}) \qquad V(\boldsymbol{r}) = -2V \sum_G \cos(\boldsymbol{G} \cdot \boldsymbol{r}_i + \phi)$$

Wu, Lovorn, Tutuc & MacDonald, PRL (2018)

Tunable Moire Bands

Energy scales: kinetic energy $E_K \sim \frac{\hbar^2}{m{a_M}^2}$ & moire potential V

Length scales: confinement length $\xi_0 \sim \left(\frac{\hbar^2 a_M^2}{mV}\right)^{\frac{1}{4}}$ & moire period a_M



$$V(\boldsymbol{r}) \approx const + \frac{1}{2}kr^2, \qquad k \sim V/a_M^2$$

a_M controls the competition between the two scales.

Tunable Moire Bands

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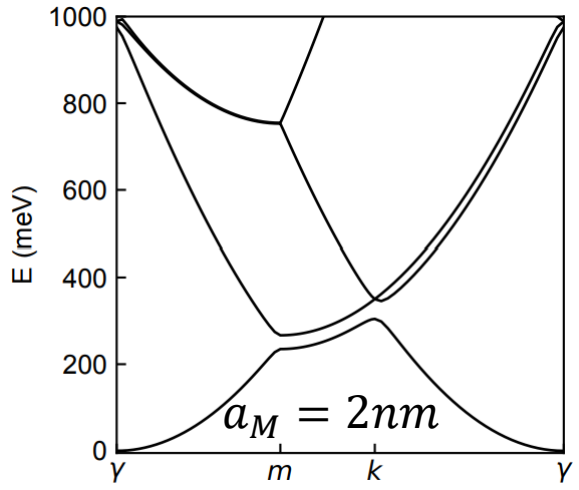
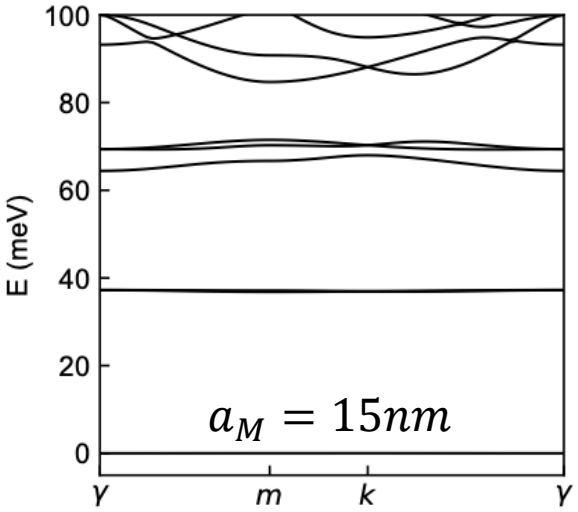
Length scales: confinement length $\xi_0 \sim \left(\frac{\hbar^2 a_M^2}{mV}\right)^{\frac{1}{4}}$ & moire period a_M

small a_M : nearly free



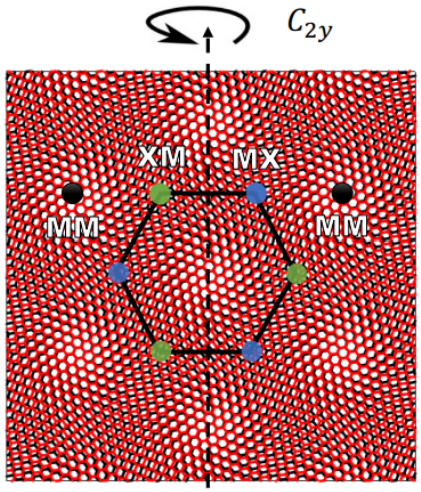
large a_M : tight binding

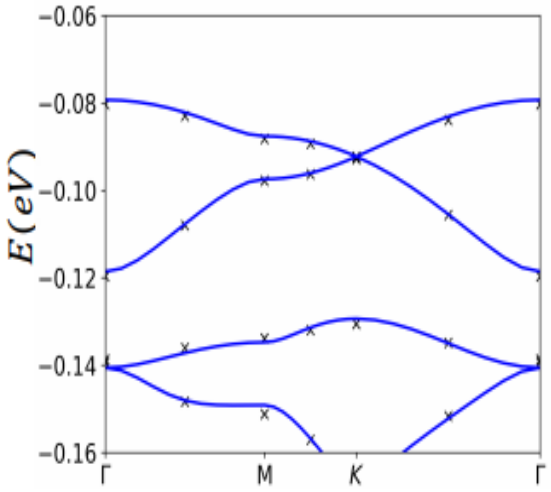


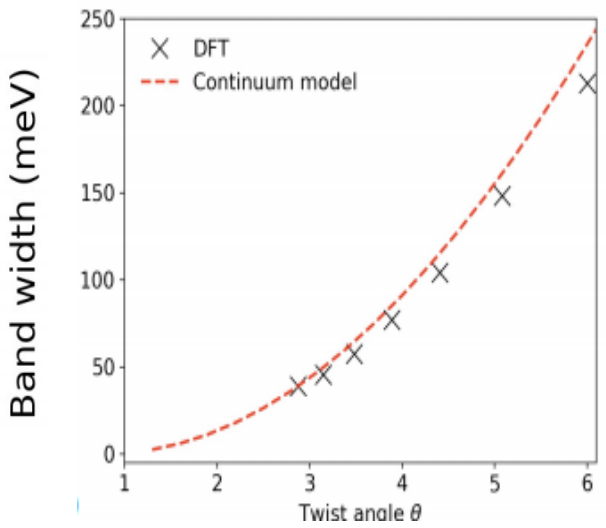
$m = 0.5me,\ \phi \sim 0,\ V =$ 15 meV for MoSe2/WSe2

Tunable Moire Bands

Twisted bilayer MoS_2 : Γ Valley, honeycomb moire lattice ($\phi = 60°$)







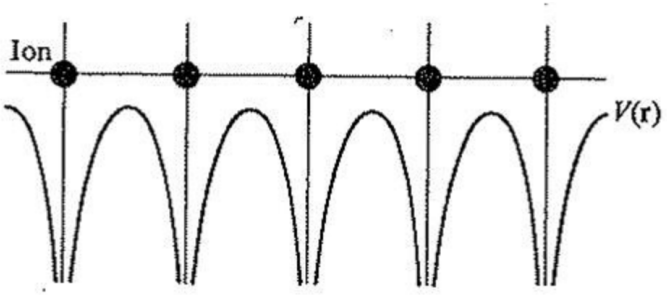
Angeli & MacDonald, PNAS (2021) Zhang, Liu & LF, PRB (2021)

Moire bandwidth decreases monotonously as $\theta \to 0$
in contrast with twisted bilayer graphene

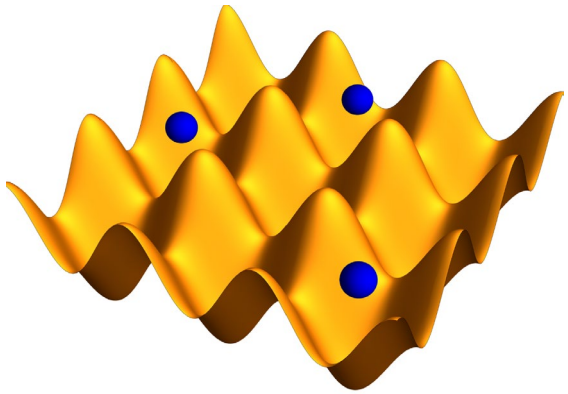
Tunable Artificial Solids

$$H = \sum_i \left(\frac{p_i^2}{2m} - V(r_i) \right) + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{\epsilon |r_i - r_j|}$$

Natural solids



Semiconductor moire



- slowly-varying, long-wavelength moire potential
- electron filling tuned by electrostatic gating

Plethora of Electron Phases

since 2020

- Mott & Charge-transfer insulators
- Generalize Wigner crystal
- Continuous metal-insulator transition
- Quantum anomalous Hall insulator
- Heavy Fermi liquid
- Light-induced magnetism & exciton Mott insulator

and many proposals: superconductivity, quantum spin liquid, spin polaron, pseudogap metal …

Outline

- Moire bands at charge neutrality (n=0)
- Single-band Hubbard model:
  Mott insulators and local moments at n=1
  electron crystals at n<1
- Two-band Hubbard model:
  charge-transfer insulators at n=1
  Mott insulator at n=2
  electron pairing from repulsion
  quantum anomalous Hall state at n=1 (Friday)
- Beyond Hubbard model:
  new theory of moire quantum matter

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Hubbard Model Physics

At large $a_M \gg \xi_0$, doped charges are tightly bound to "moire sites" defined by superlattice potential minima, leading to a **periodic array of artificial atoms** that are weakly coupled by electron tunneling and interaction.

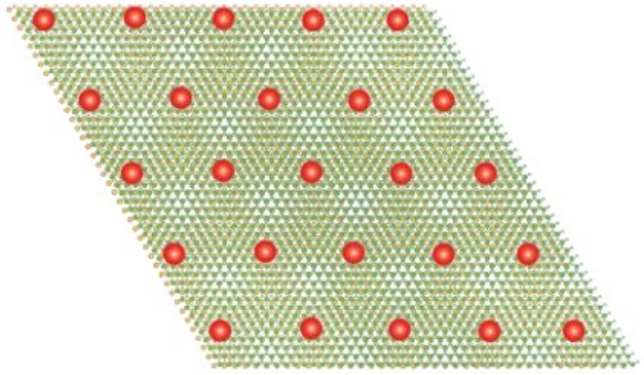
Effective Hubbard model*: $H = -t\sum c_i^+ c_j + U_{ij} n_i n_j$

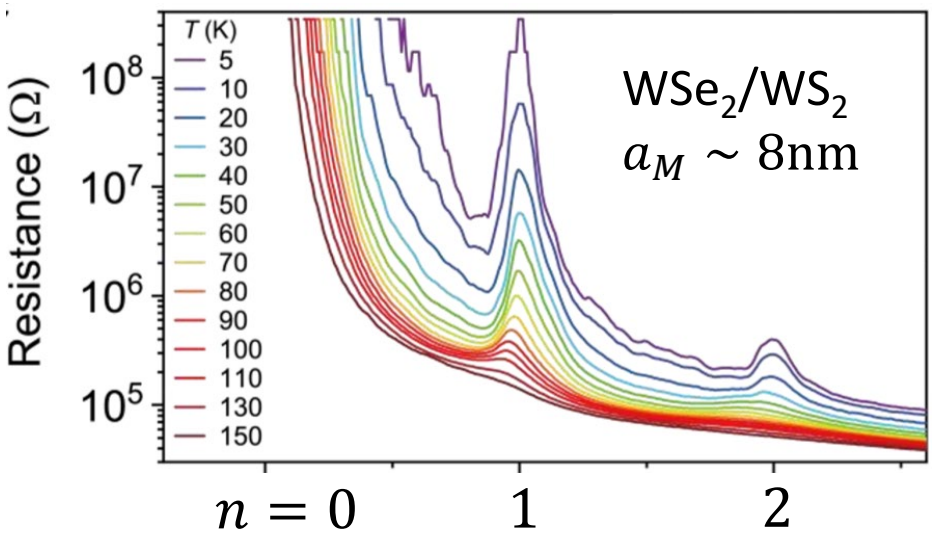
Hierarchy of energy scales: Wu et al, PRL (2018)

$$U \sim \frac{e^2}{\epsilon \xi_0} \gg V \sim \frac{e^2}{\epsilon a_M} \gg t \sim \exp\left(-\frac{a_M}{\xi_0}\right)$$

* its applicability regime will be examined later.

Mott Insulator



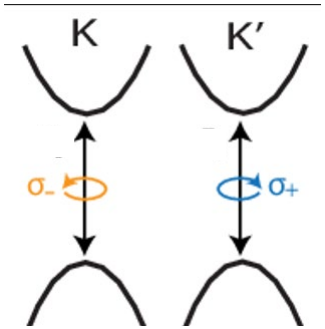


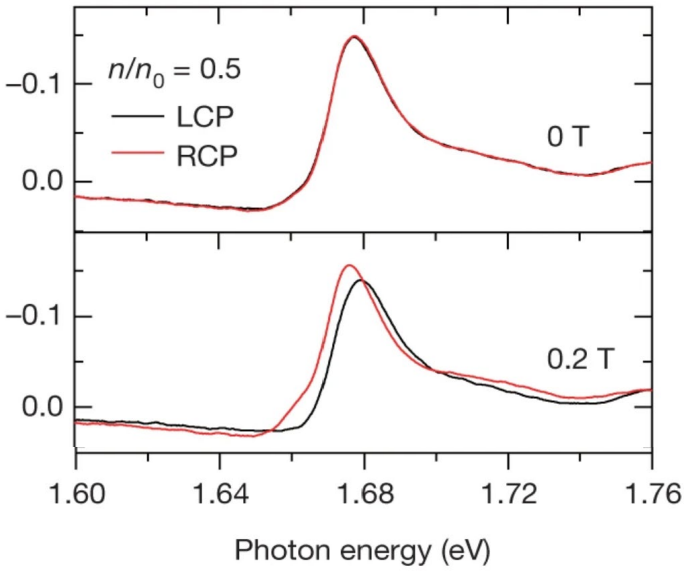
Tang et al, Nature (2020)

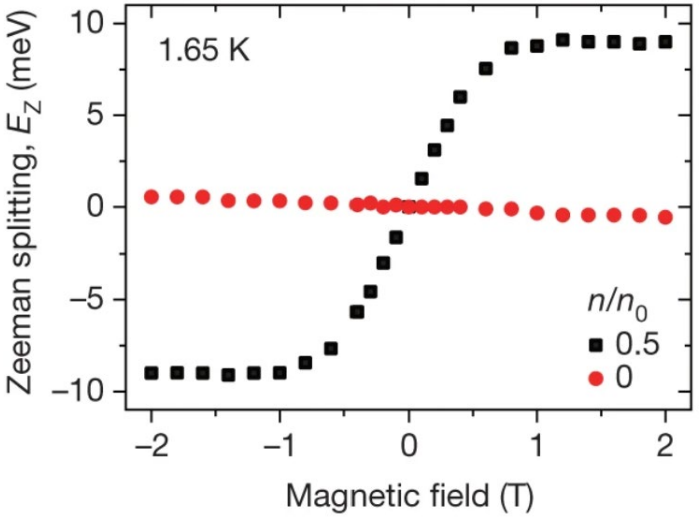
Regan et al, Nature (2020)

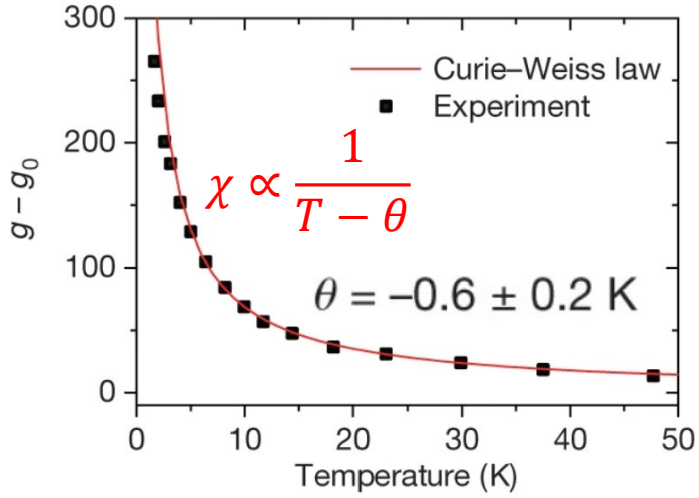
Electron hopping is prohibited by strong on-site repulsion U

Antiferromagnetic Exchange Interaction





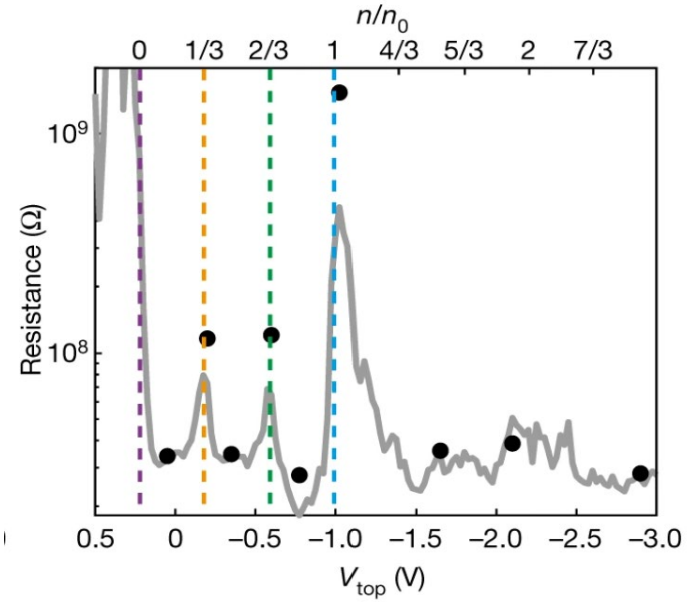




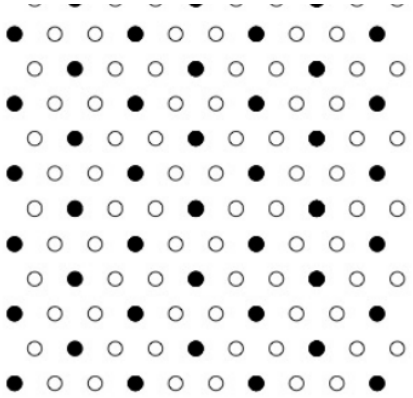
Tang et al, Nature (2020)

Generalized Wigner Crystals

- $t \to 0$ limit: interacting classical charges on triangular lattice
- Coulomb interactions produce *incompressible* electron crystals at commensurate fractional fillings.

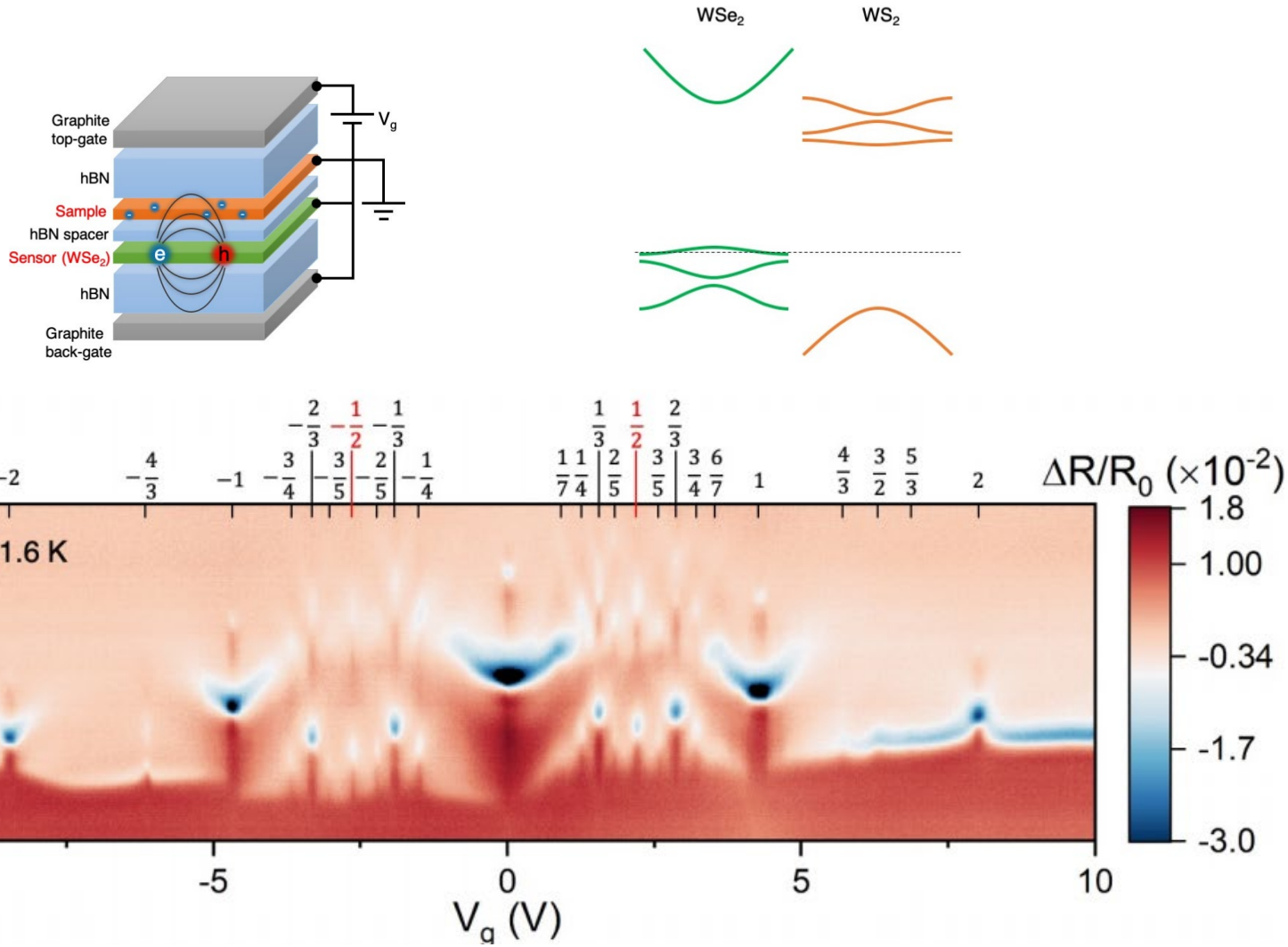


Regan et al, Nature (2020)



$$n = \frac{1}{3}, \frac{2}{3}$$

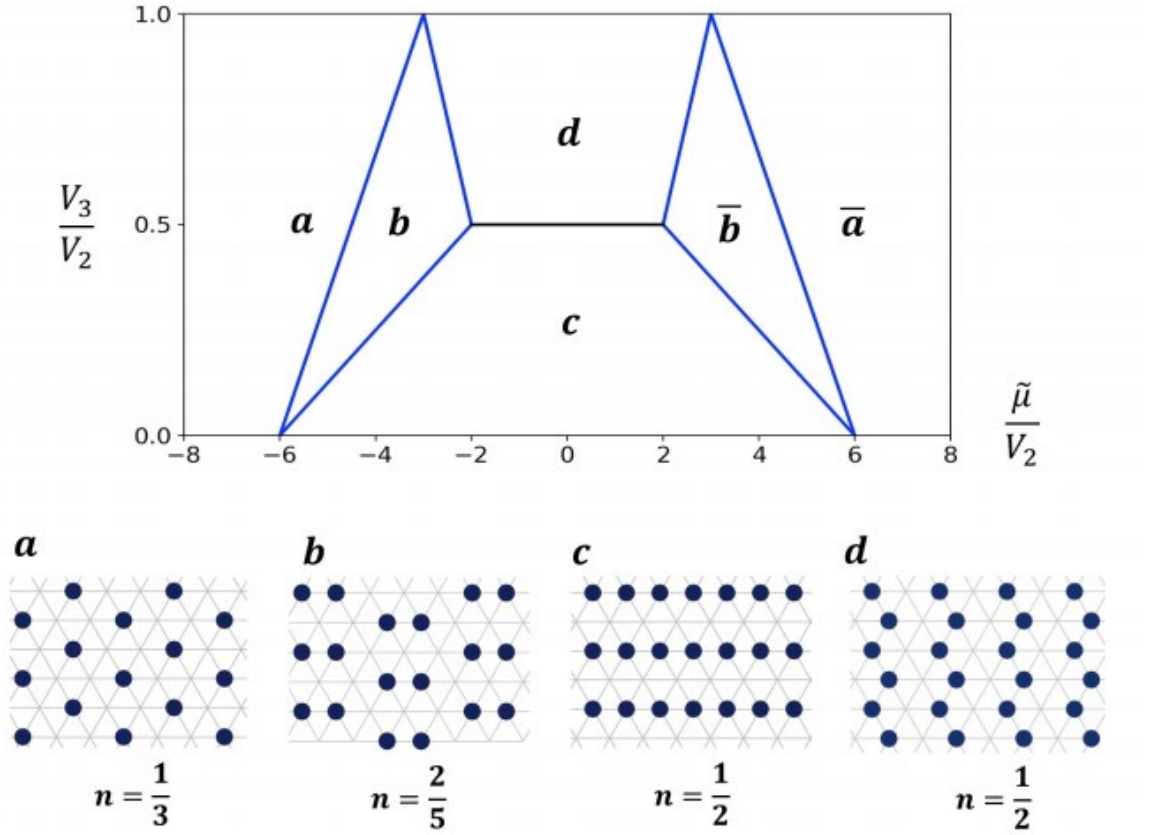
Generalized Wigner Crystals

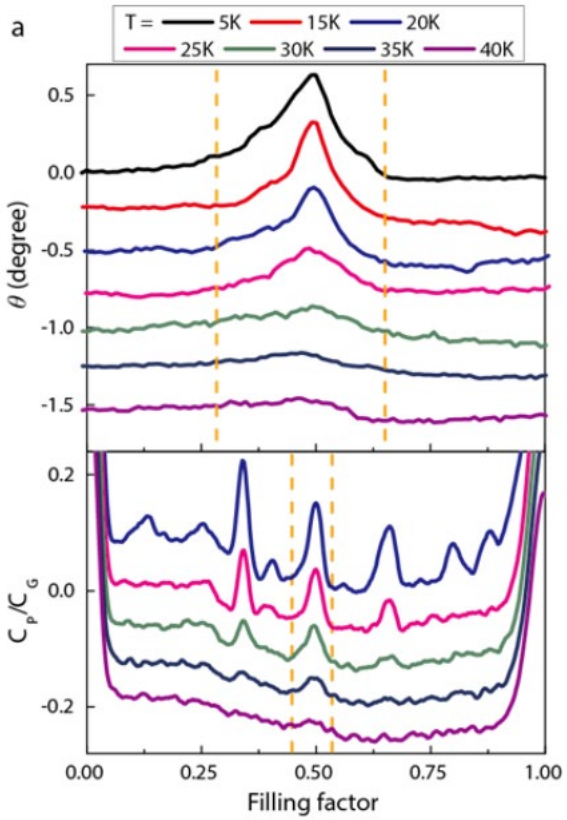


Xu et al, Nature (2020)

Stripe Wigner Crystals

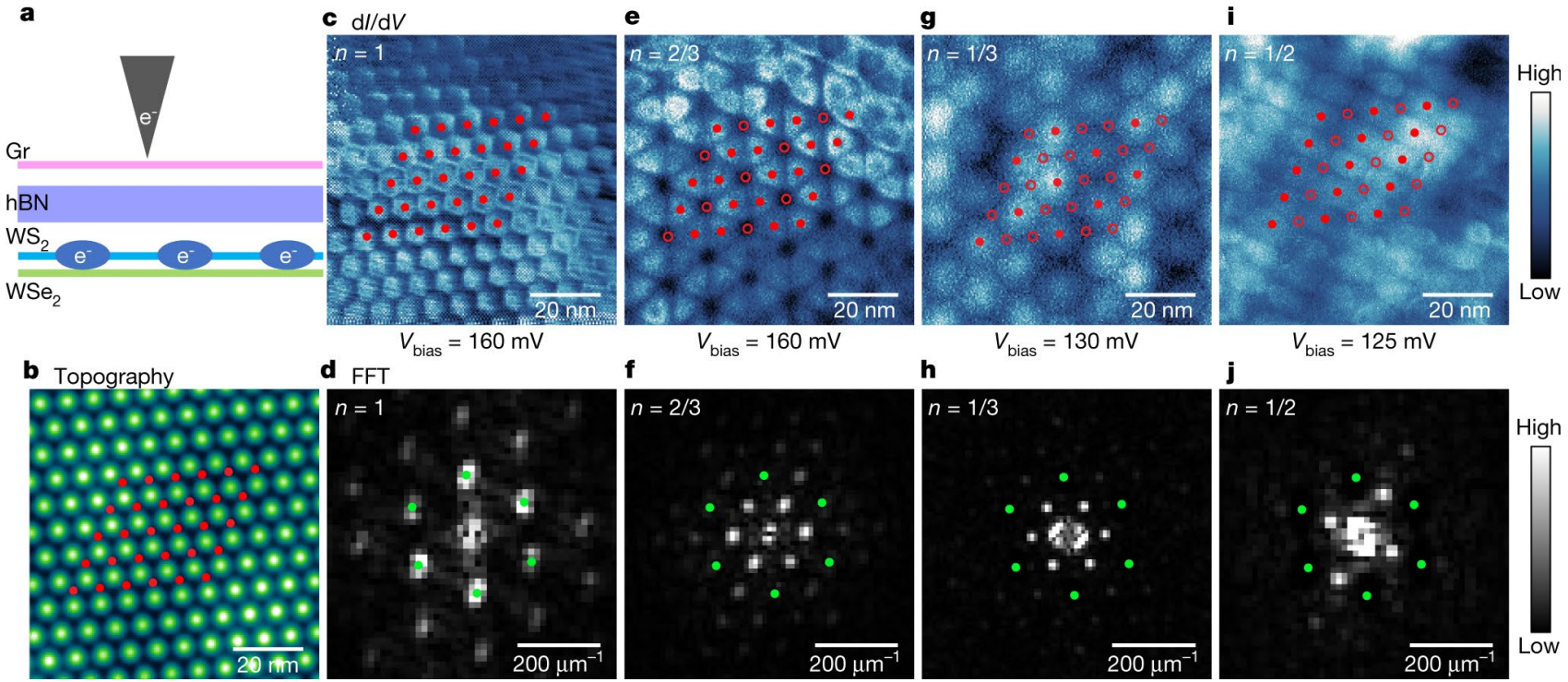
Phase diagram of triangular lattice gas with V_1, V_2, V_3





Cornell + MIT, Nature Materials (2021)

Imaging Electron Crystals



Li et al, Nature (2021)

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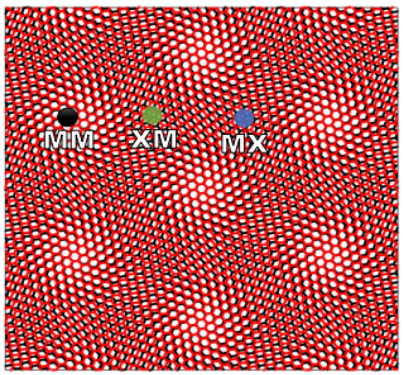
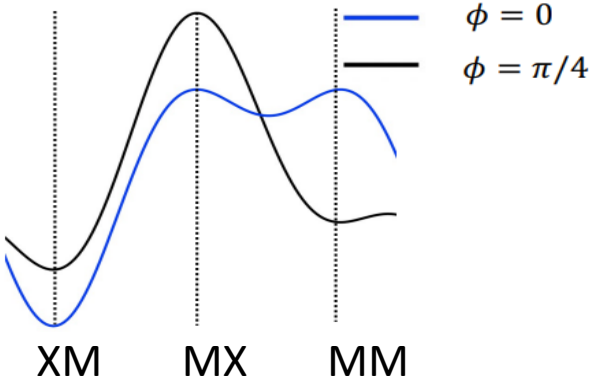
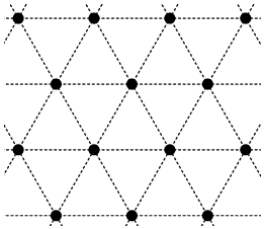
Moire Potential Landscape

$$V(\boldsymbol{r}) = -2V_0 \sum_G \cos(\boldsymbol{G} \cdot \boldsymbol{r}_i + \phi)$$

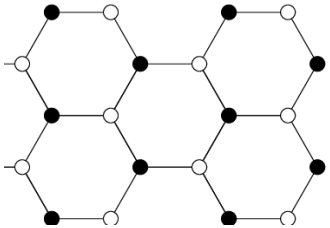




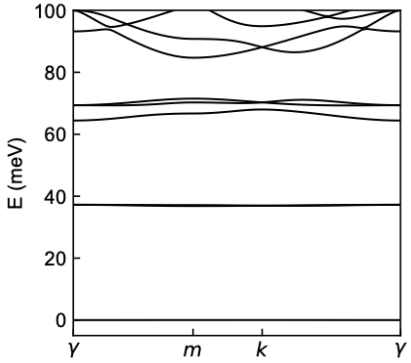
$\phi \in (0, \frac{\pi}{6})$:



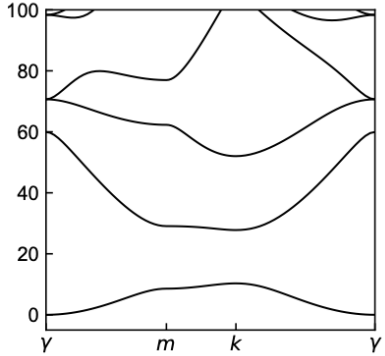
$\phi \in (\frac{\pi}{6}, \frac{\pi}{3})$:



$MoSe_2/WSe_2$



WSe_2/WS_2

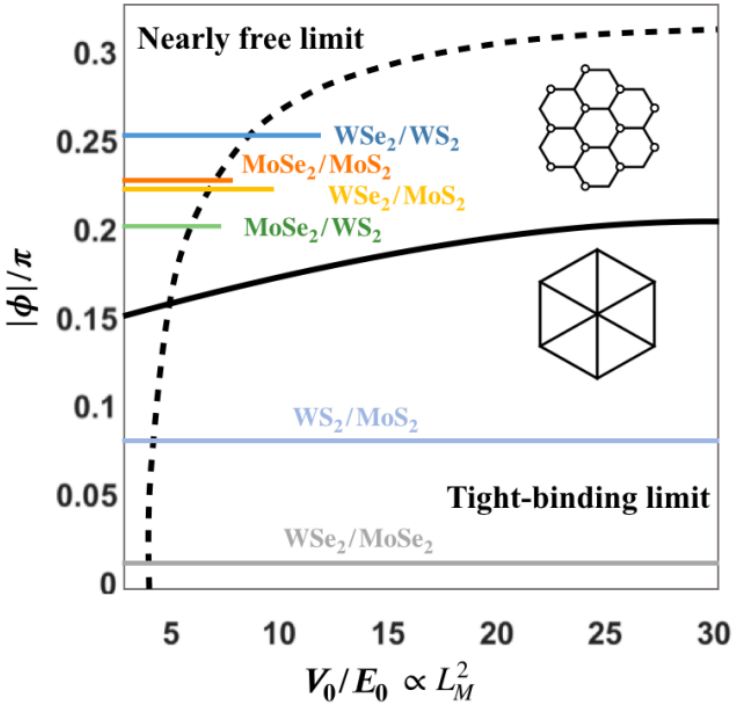


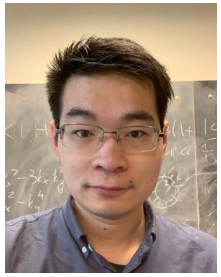
Zhang, Yuan & LF, PRB (2020)

Semiconductor Heterostructures

From large-scale DFT:

System	δ	ΔE_g	V_0	ϕ	$E_0^{\min}$
WSe_2/WS_2	4%	640	15	45°	1.2
WSe_2/MoS_2	4%	940	11	40°	1.2
$MoSe_2/MoS_2$	4%	630	9	42°	1.3
$MoSe_2/WS_2$	4%	270	7	35°	1.3



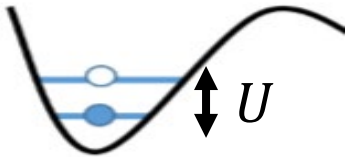


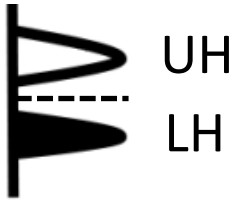
Yang Zhang

Zhang, Yuan & LF, PRB (2020)

Charge-Transfer Insulator

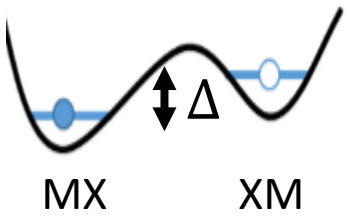
Mott-Hubbard insulator

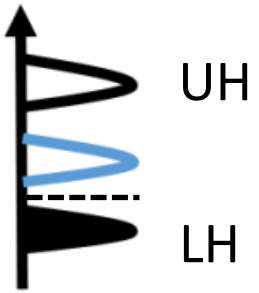




$U > \Delta$:
Charge transfer insulator

(similar to CuO_2)



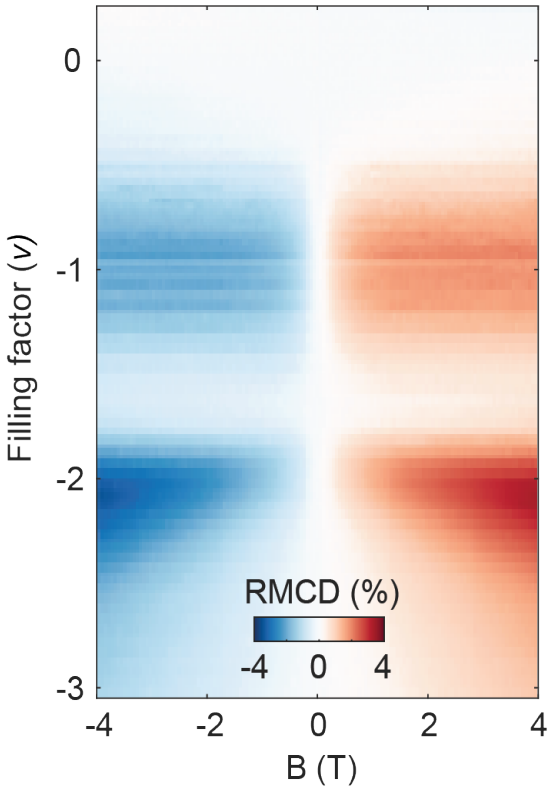


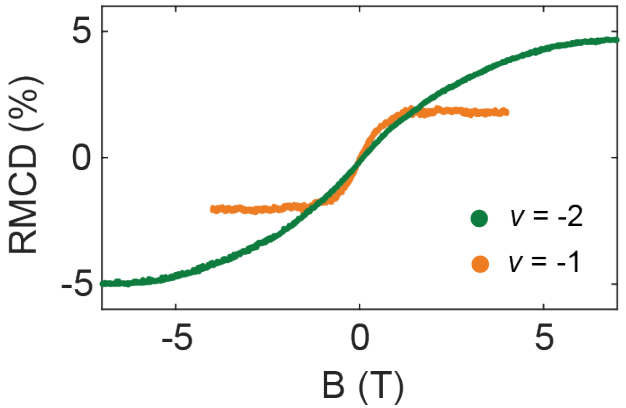
- doped charges at n>1 occupy secondary minima to avoid U.
- insulating gap at n=1 set by Δ

Zhang, Yuan & LF, PRB (2020)

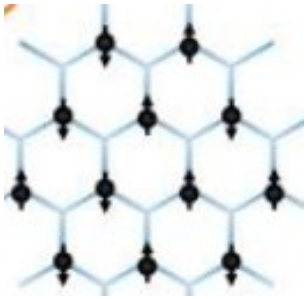
Charge Transfer at $1 < n \leq 2$

WSe_2/WS_2



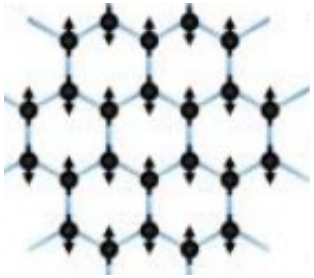


$n = 1$



charge-transfer
Mott insulator

$n = 2$



honeycomb lattice
Mott insulator

Xiaodong Xu et al (submitted)

Xu et al, arXiv:2202.02055

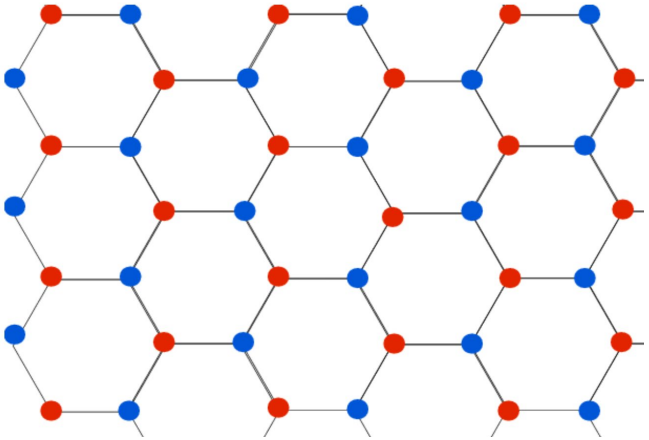
Doping Charge Transfer Insulator

Hubbard model with extended repulsion on honeycomb lattice with staggered potential

$$H = H_0 + H_t$$

$$H_0 = \Delta \sum_{r \in B} n_r + \sum_{r,r'} V_{rr'} n_r n'_r$$

$$H_t = -t \sum_{\langle rr' \rangle} (c_r^\dagger c_{r'} + hc.)$$



Slagle & LF, PRB (2020)

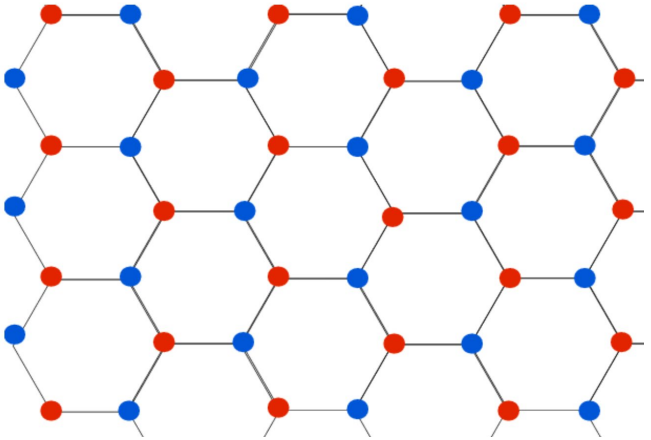
Strong Coupling Limit

$t \to 0$ limit: interacting classical charges on the lattice

$$H = H_0 + H_t$$

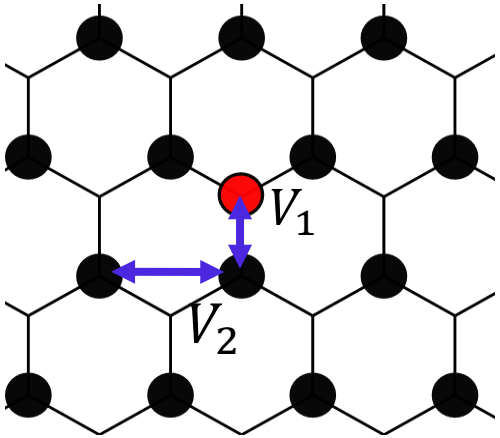
$$H_0 = \Delta \sum_{r \in B} n_r + \sum_{r,r'} V_{rr'} n_r n'_r$$

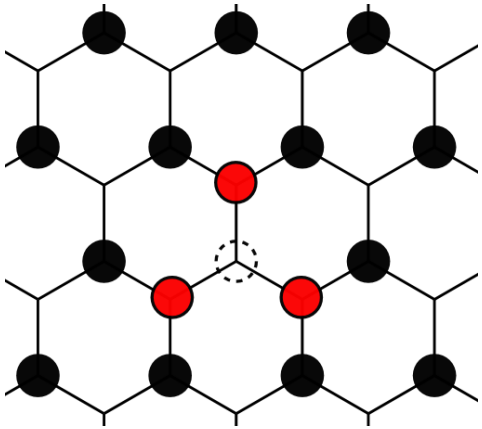
$$H_t = -t \sum_{\langle rr' \rangle} (c_r^\dagger c_{r'} + hc.)$$



Attraction by Repulsion!

Classical electrostatics effect



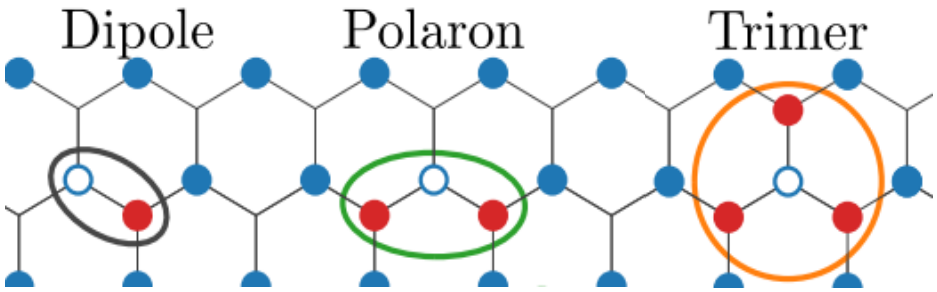


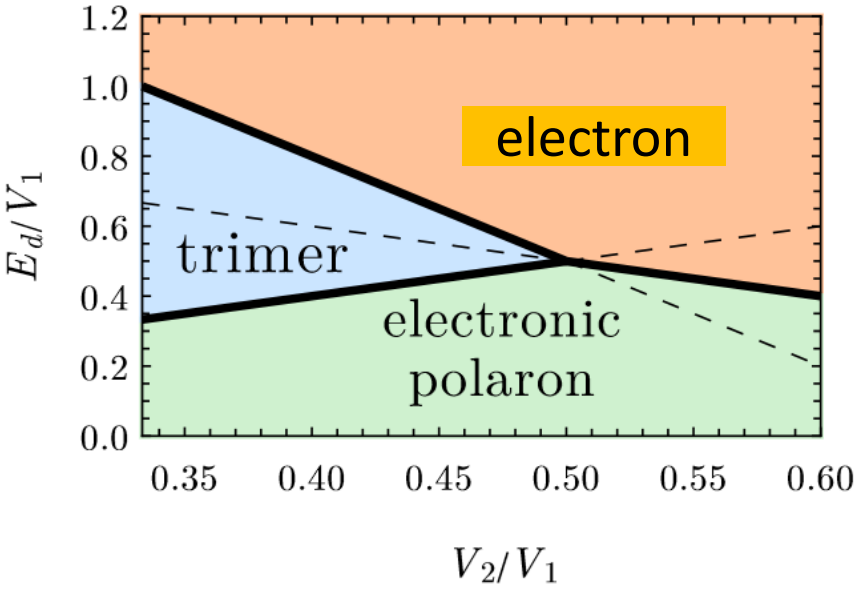
$$E_t = 2E_1 + \Delta - 3V_2$$

For $\Delta < 3V_2$, a charge-2e "trimer" has lower energy than two separate electrons!

Slagle & LF, PRB (2020)

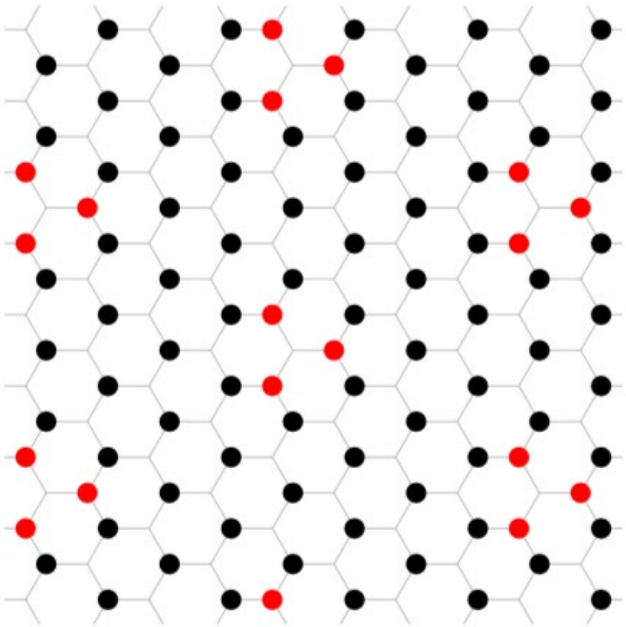
Charge Excitations



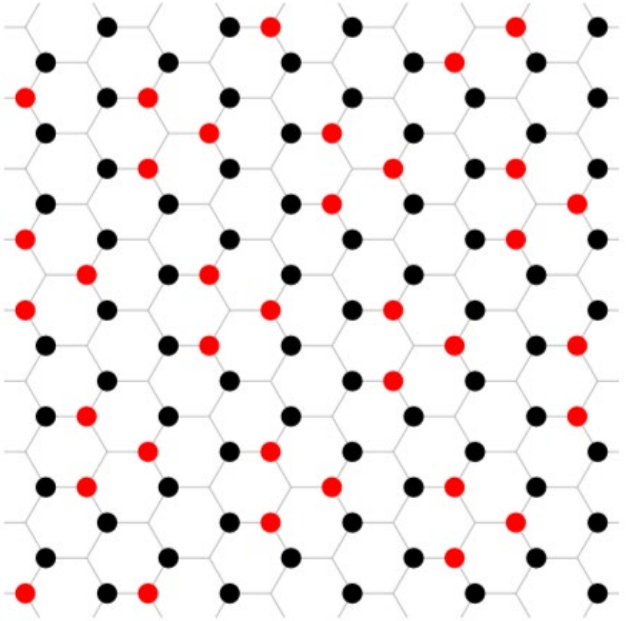


- E_d: energy of a dipole
  $E_d = \Delta + 2V_1 - 6V_2 + \cdots$
- Phase diagram accounts for **all** V_{ij}
- doped charges may exist as electron, polaron, or charge-2e trimer.

Pair Density Waves



(b) $\delta = 1/8 = 0.125$



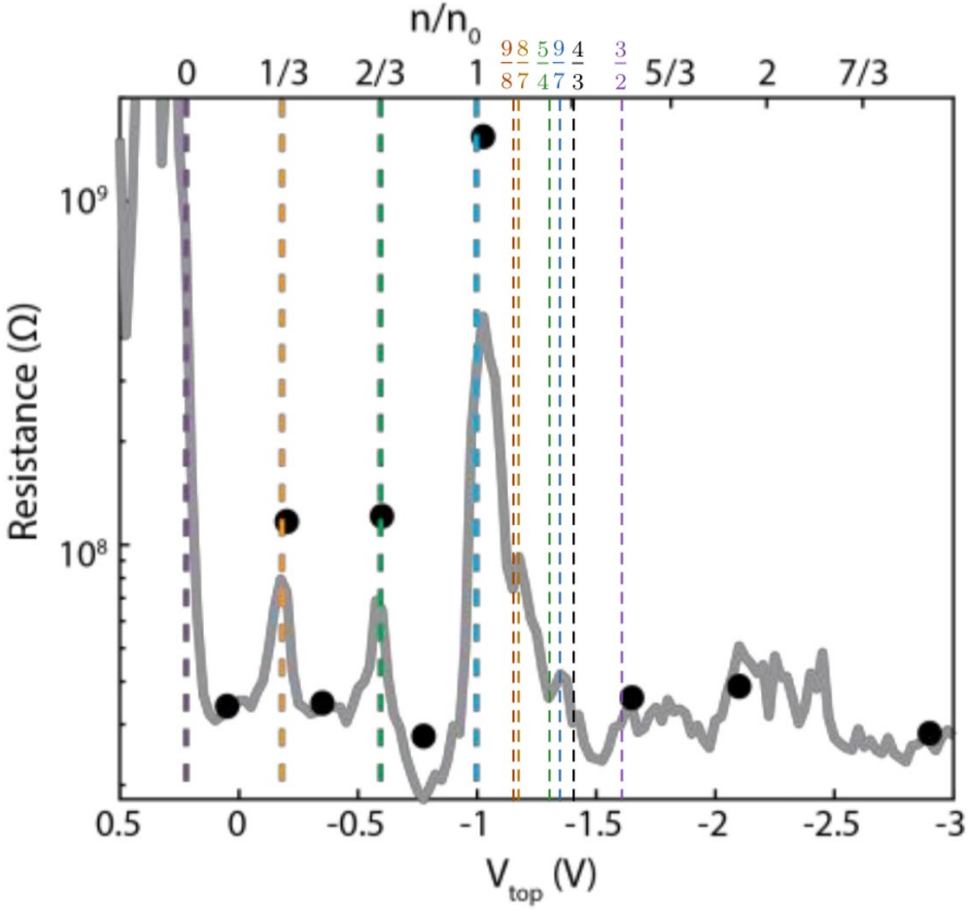
(d) $\delta = 2/7 \approx 0.286$

densest packing of trimers for $V_{n\leq 4}$

contrasts with electron crystals at $\delta = 1/3$ and $1/4$

Slagle & LF, PRB (2020)

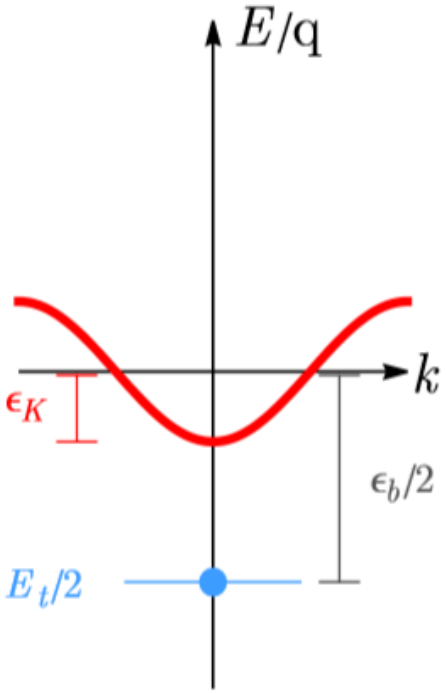
Hint of Electron Trimers at n>1 ?

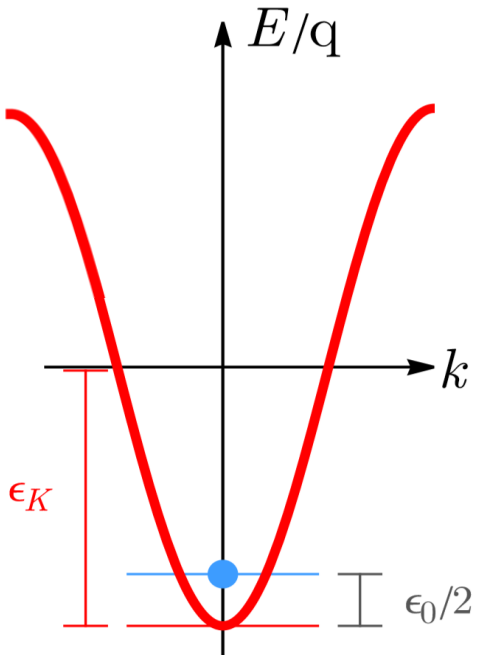


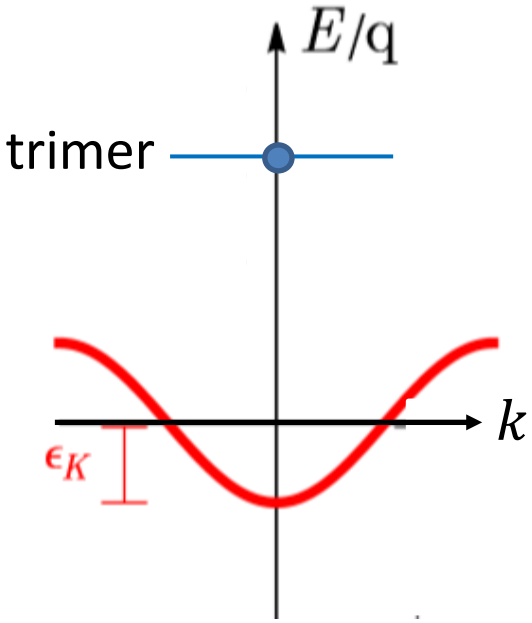
Regan, Nature (2020)

STM image of charge configuration needed

Trimer Enabled Superconductivity







Pair density wave

Resonant SC

$E_t - 2E_1 = \Delta - 3V_2 \gg t$

Slagle & LF, PRB (2020)

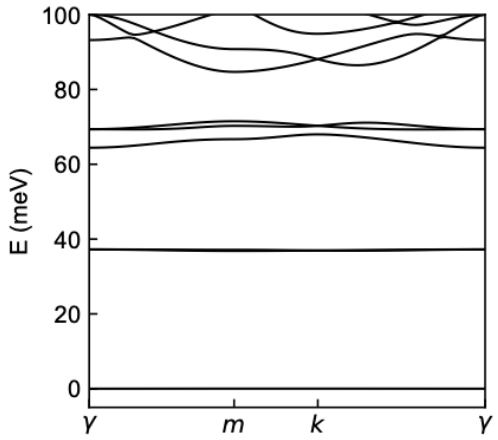
Crepel & LF, Science Advances (2021)

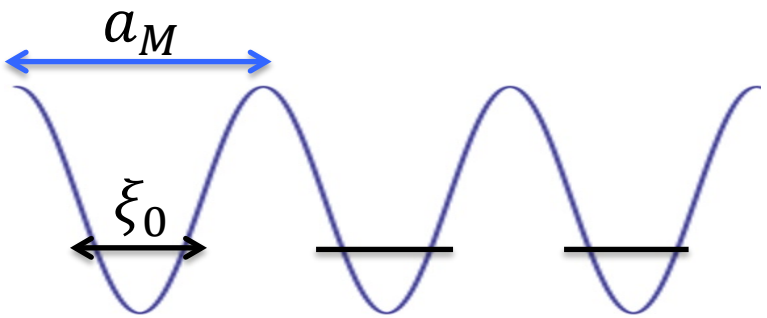
Outline

- Moire bands at charge neutrality (n=0)
- Single-band Hubbard model:
  Mott insulators and local moments at n=1
  electron crystals at n<1
- Two-band Hubbard model:
  charge-transfer insulators at n=1
  Mott insulator at n=2
  electron pairing from repulsion
  quantum anomalous Hall state at n=1 (Friday)
- Beyond Hubbard model: Reddy, Devakul & LF, arXiv:2301.0079
  new theory of moire quantum matter

Applicability Regime of Hubbard Model

Hubbard models (with nonlocal interaction) are obtained by projection to the lowest moire band.





At large a_M, $\xi_0 \propto \sqrt{a_M} \ll a_M$

Red Herring: on-site interaction thus obtained $U \sim \frac{e^2}{\epsilon \xi_0} \propto a_M^{-\frac{1}{2}}$ is parametrically larger than the band gap $\hbar\omega \sim \sqrt{\frac{V}{m a_M^2}}$ as $a_M \to \infty$.

A New Length Scale

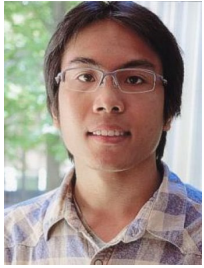
Moire atom = quantum dot: $V(\boldsymbol{r}) \approx \frac{1}{2} k r^2$, with $k \sim V/a_M^2$

Size of electron molecule in classical limit (Wigner molecule)

$$\xi_c \equiv \left(\frac{e^2}{2\epsilon k}\right)^{1/3} \propto a_M^{2/3} \qquad \lambda \equiv \frac{e^2/\epsilon\xi_0}{\hbar\omega} = 2(\xi_c/\xi_0)^3$$

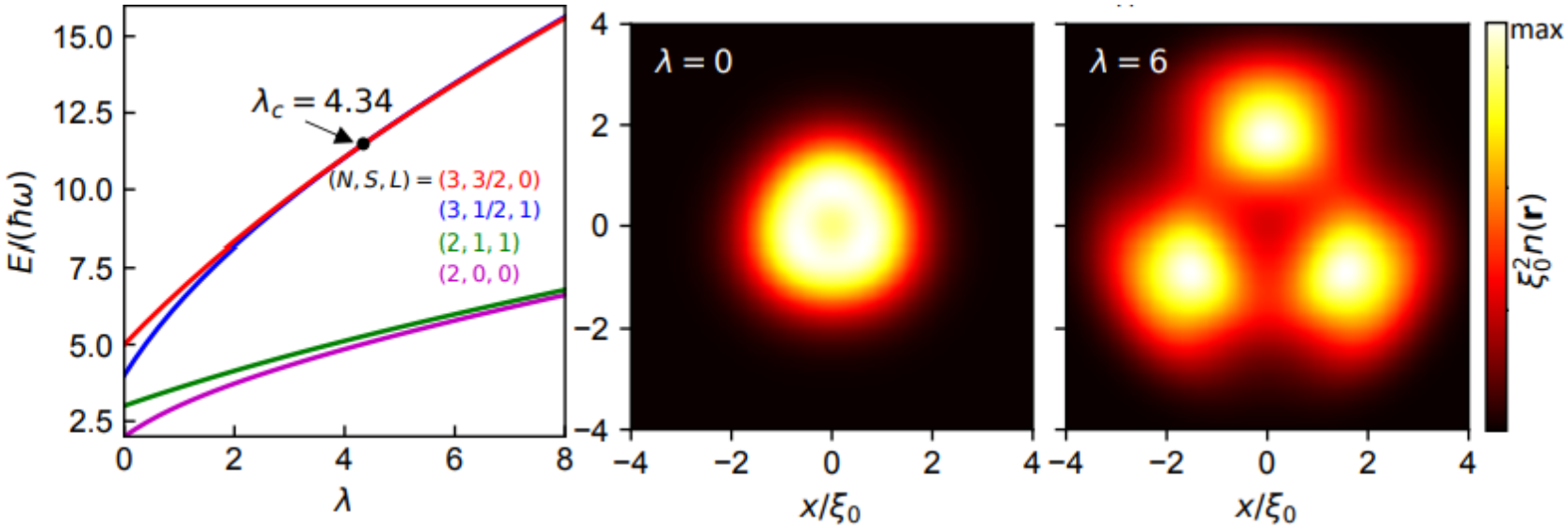
At large moire period, the hierarchy of length scales:

$$a_M > \xi_c > \xi_0$$

Moire Atoms

strong coupling regime at large a_M

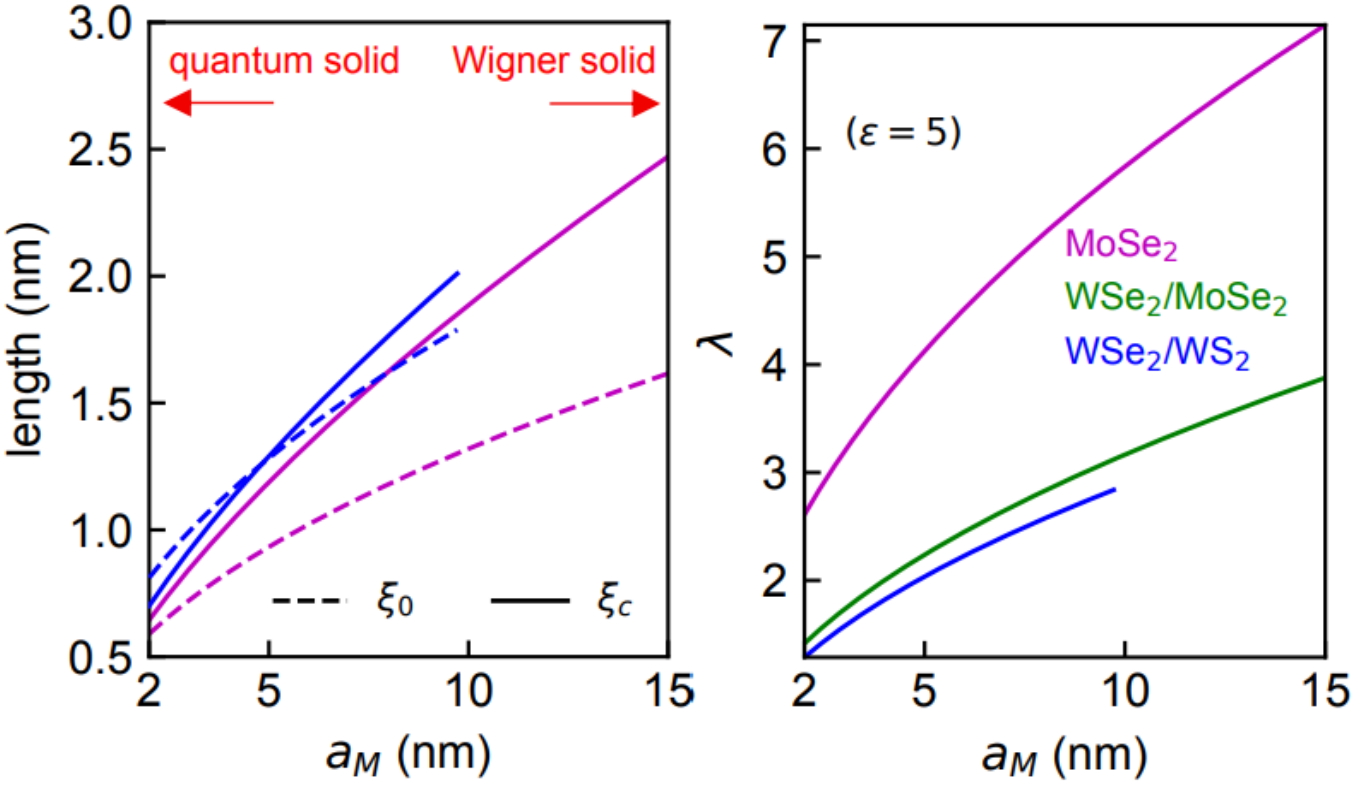


- Two-electron atom: GS deviates strongly from Slater determinant;

  $E_2 - 2E_1 \equiv U < \frac{e^2}{\epsilon \xi_0}$

- Three-electron atom: low-high spin transition at B=0; crystal field stabilizes Wigner molecule.

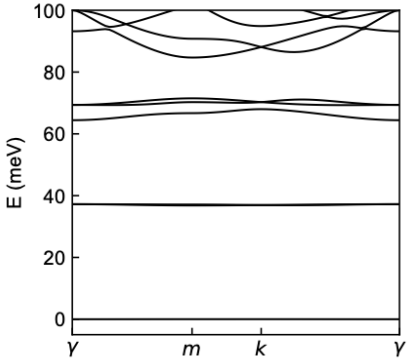
From Moire Atoms to Moire Solids



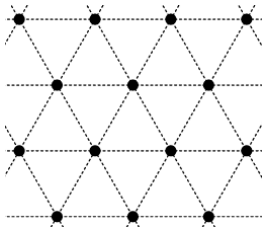
Moire Solids

Effective Hilbert space changes strongly with filling

$n = 0$

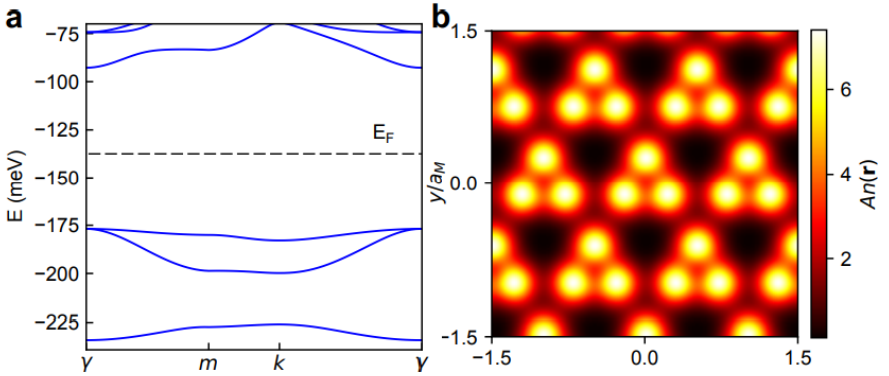


$n = 1$



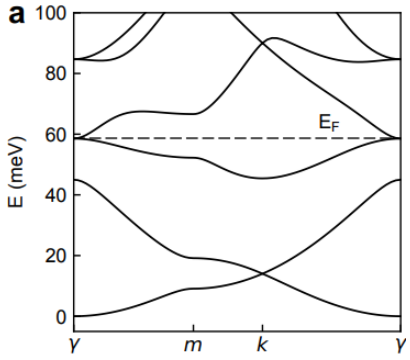
triangular

$n = 3$

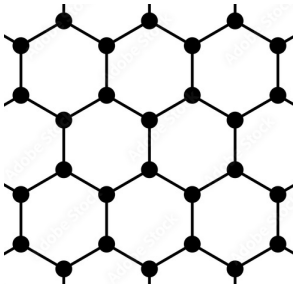


Kagome

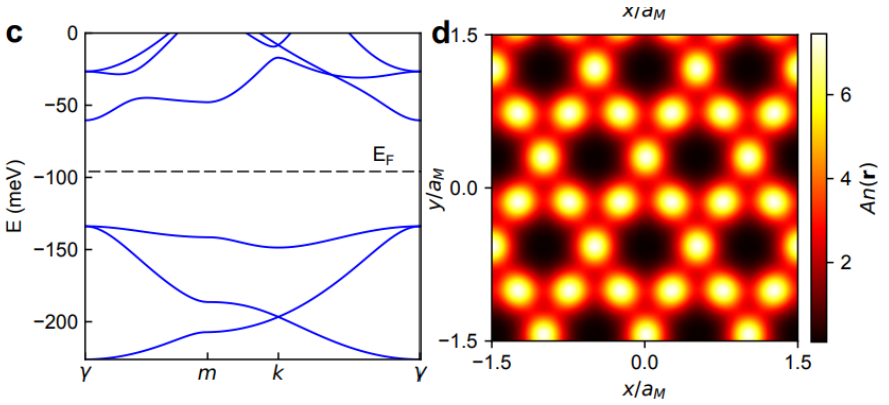
$n = 0$



$n = 2$



honeycomb



Strong Interaction in Semiconductor Moires

- Mott insulators and local moments at n=1
- electron crystals at n<1
- charge transfer between 1<n<=2

  electron pairing from repulsion
- strong-coupling regime of moire quantum matter

Theory

Yang Zhang

Noah Yuan

Bi Zhen

Hiroki Isobe

Trithep Devakul

Philip Crowley

Nisarga Paul

Valentin Crepel

Margarita Davydova

Aidan Reddy

Kevin Slagle (Caltech)

Junkai Dong (Cornell)

Jie Wang (Flatiron)

Experiment

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Feng Wang (Berkeley)

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Ben Feldman (Stanford)

Pablo Jarillo-Herrero

SIMONS FOUNDATION