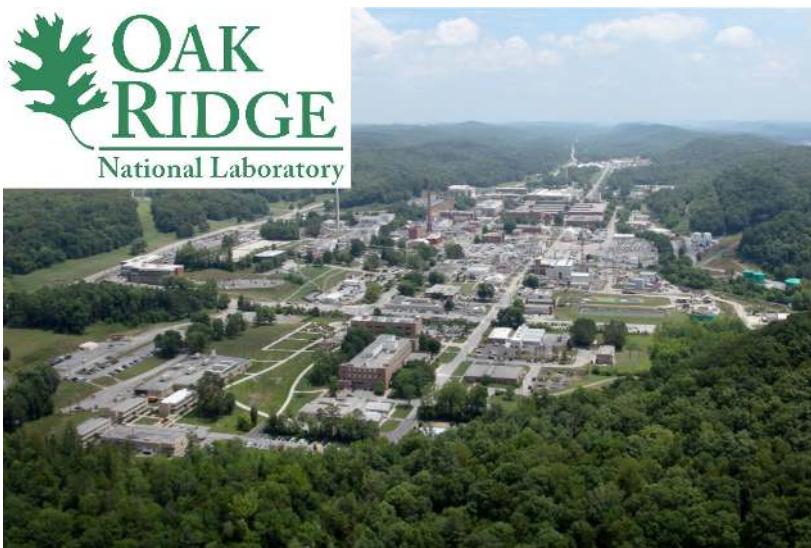


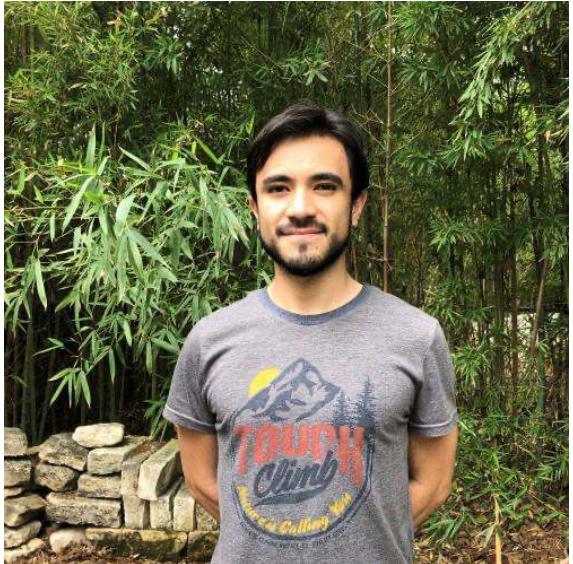
Magnetic ground states of honeycomb lattice Wigner crystals

Nitin Kaushal

Oak Ridge National Lab



Collaborators:



Nicolas-Morales Duran
University of Texas at
Austin, USA.



Prof. Allan H. MacDonald
University of Texas at
Austin, USA.



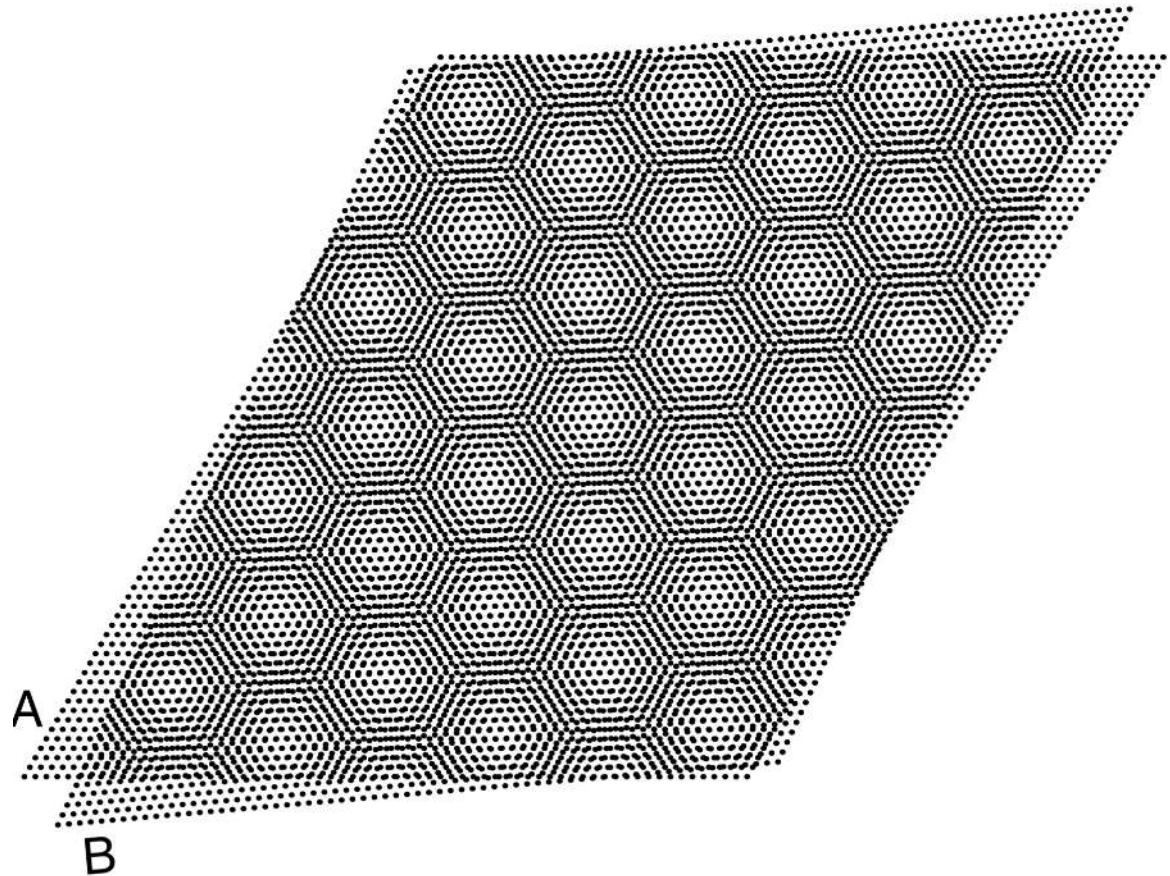
Prof. Elbio Dagotto
University of Tennessee,
Knoxville, USA.
Oak Ridge National Lab,
USA.

Outline:

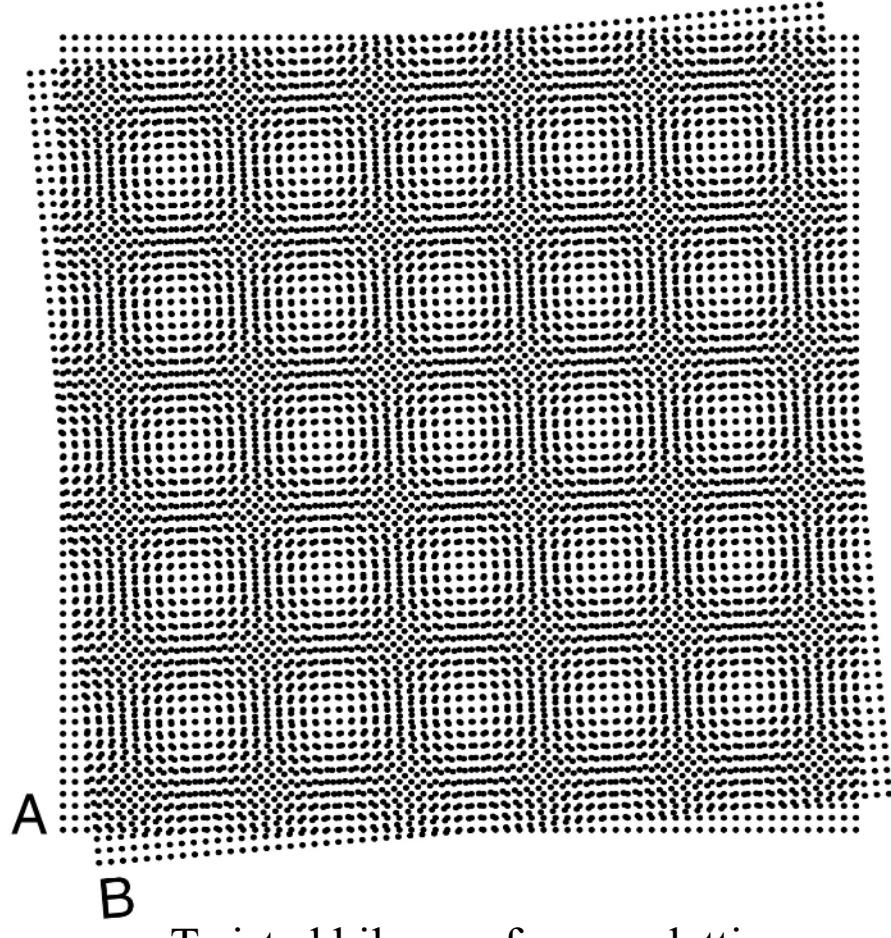
- Introduction to moiré superlattice.
- Moiré bands in homobilayers of gamma-valley Transition Metal Dichalcogenides (TMD).
- Lattice Hamiltonian.
- Results using unrestricted Hartree-Fock technique.
- Conclusion.

Moiré superlattice:

created using multiple planes



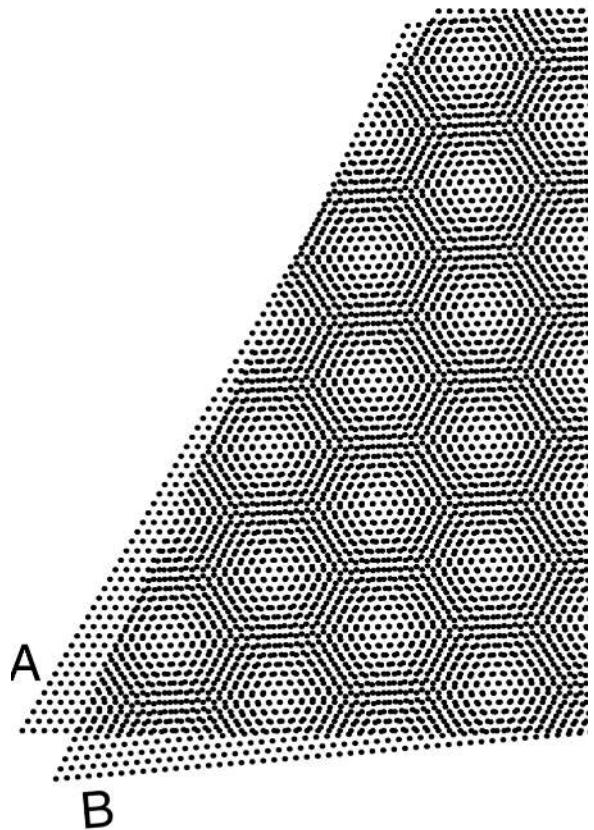
Twisted bilayer of triangular lattices



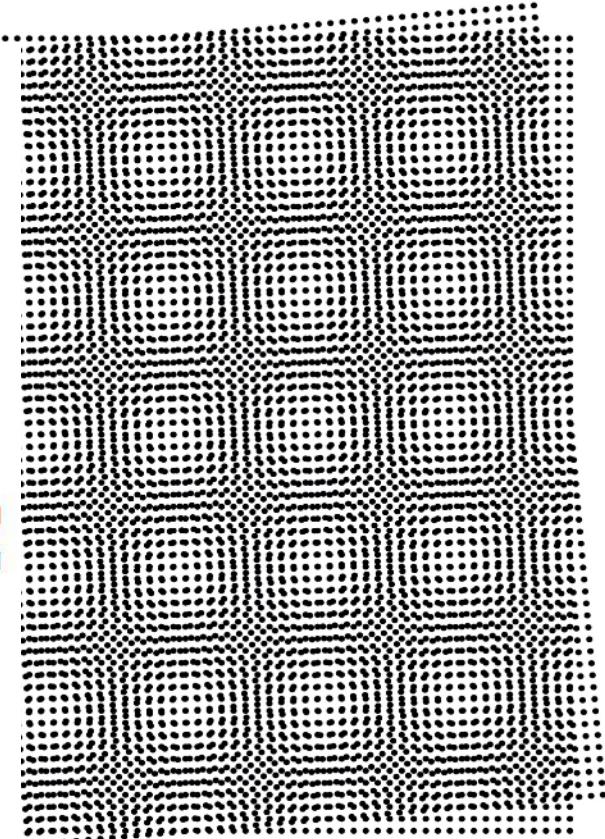
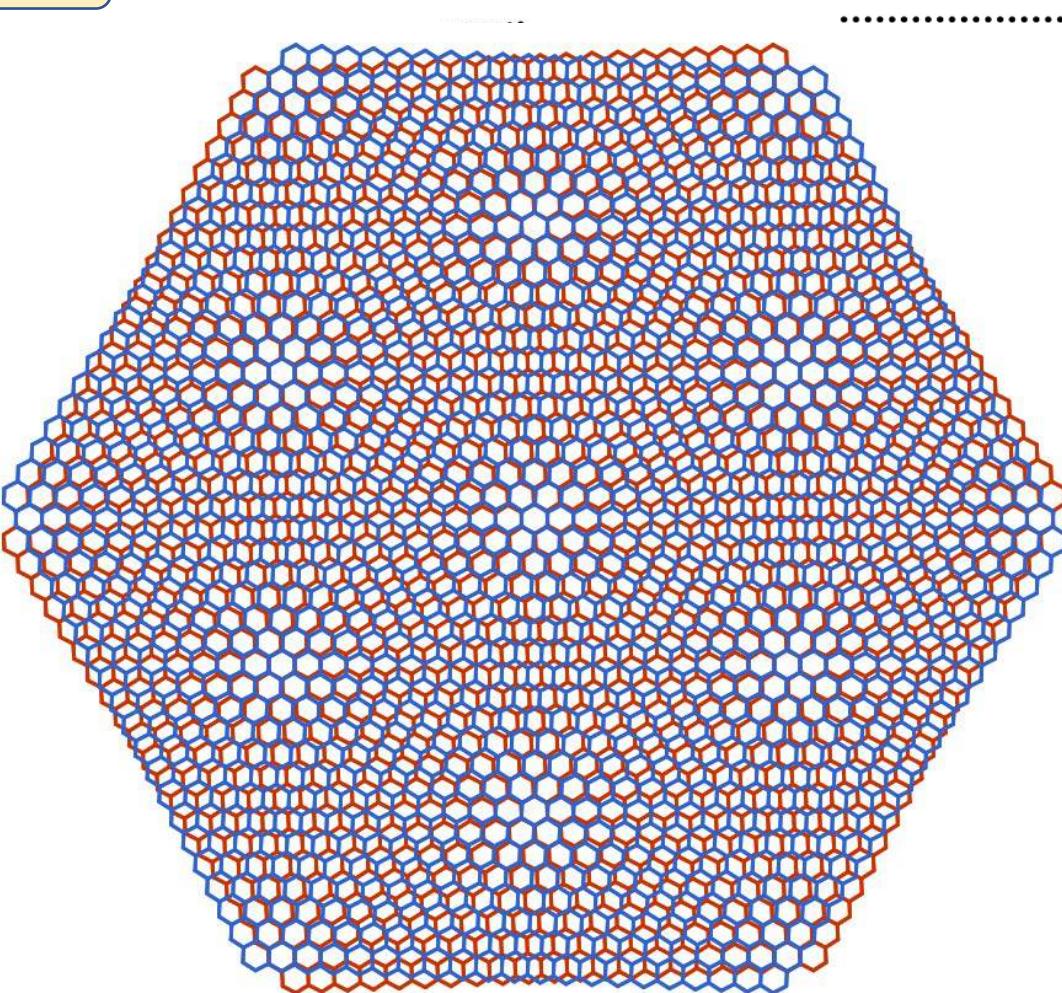
Twisted bilayer of square lattices

Moiré superlattice:

created using multiple planes



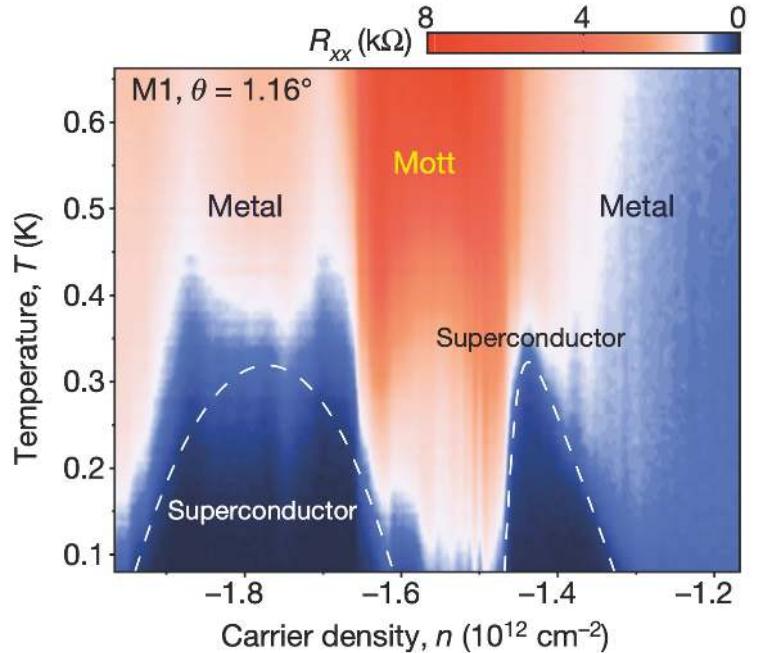
Twisted bilayer of trian



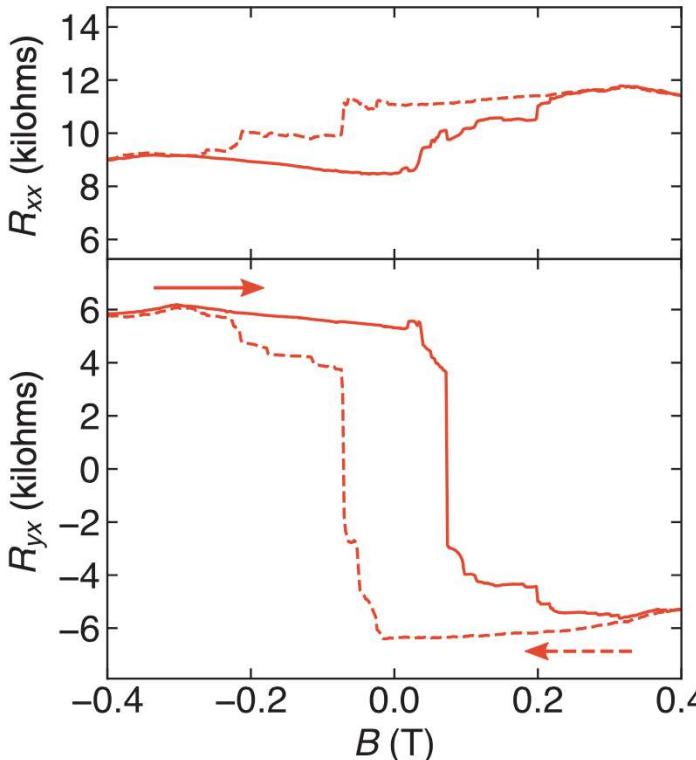
1 bilayer of square lattices

Twisted bilayer graphene

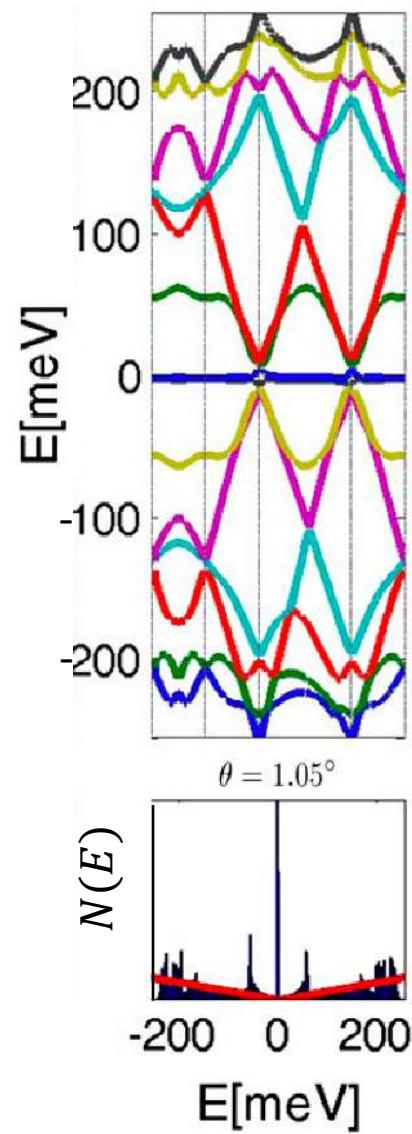
- Mott insulator at half-filling
- Strongly correlated superconductivity near half-filling
- Ferromagnetism for three-quarter filling



Easily tunable carrier filling via gate voltage. \leftrightarrow !!



All interesting physics near magic angle $\sim 1.05^\circ$, where flat bands are found.



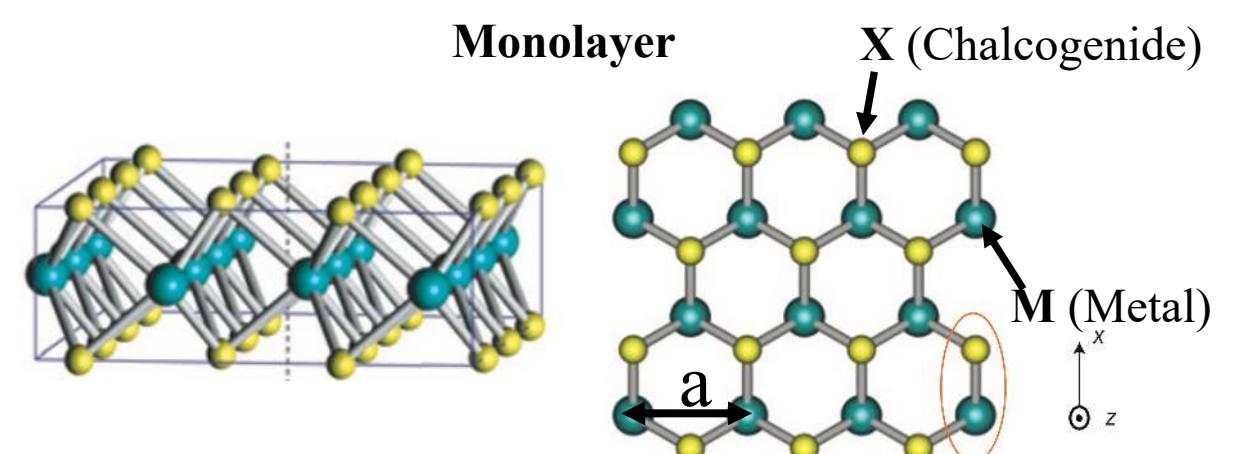
G. Li, et al. Nature Phys. **6**, 109-113 (2010).

R. Bistritzer and A. H. MacDonald, Proc. Natl. Acad. Sci. USA **108**, 12233 (2011).

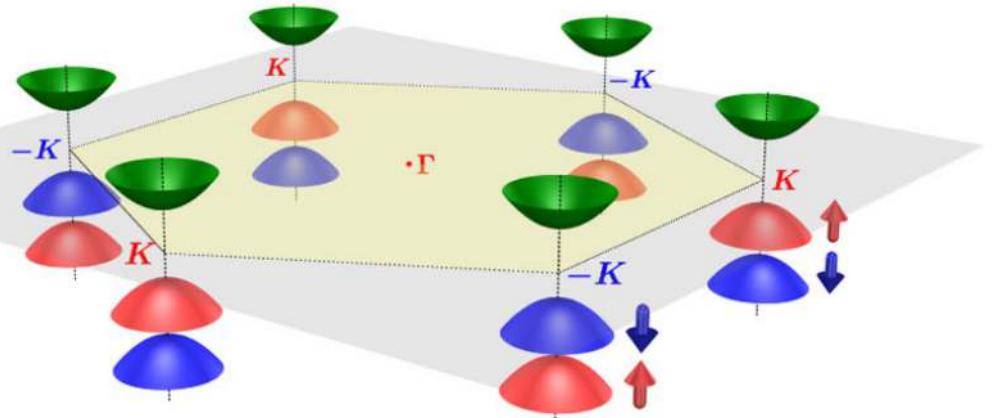
Y. Cao, et al. Nature **556**, 43–50 (2018) and Nature **556**, 80–84 (2018).

A. L. Sharpe, et al. Science **365**, 605–608 (2018).

TMD (MX_2) moiré lattices

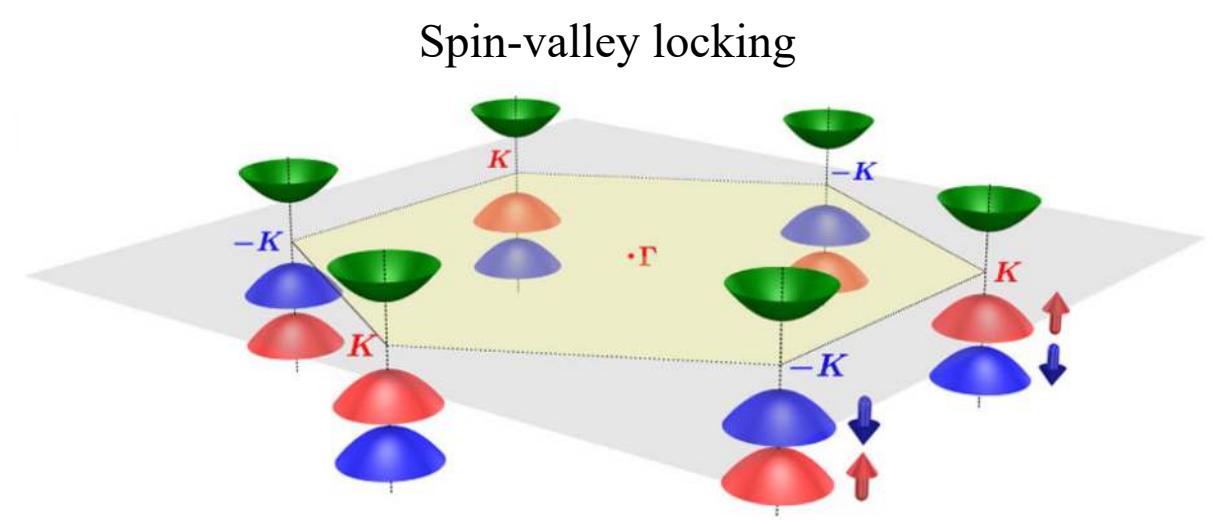
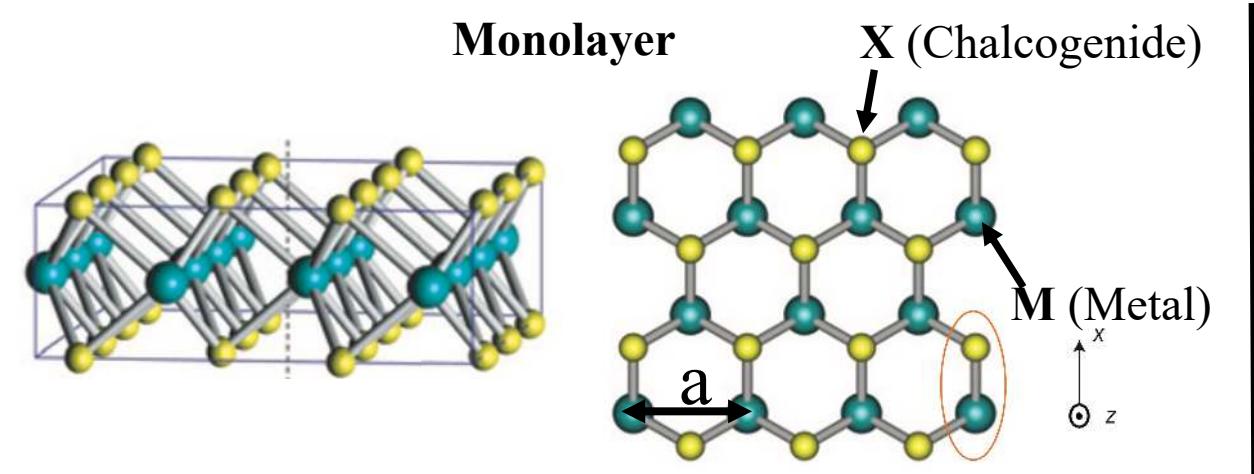


Spin-valley locking

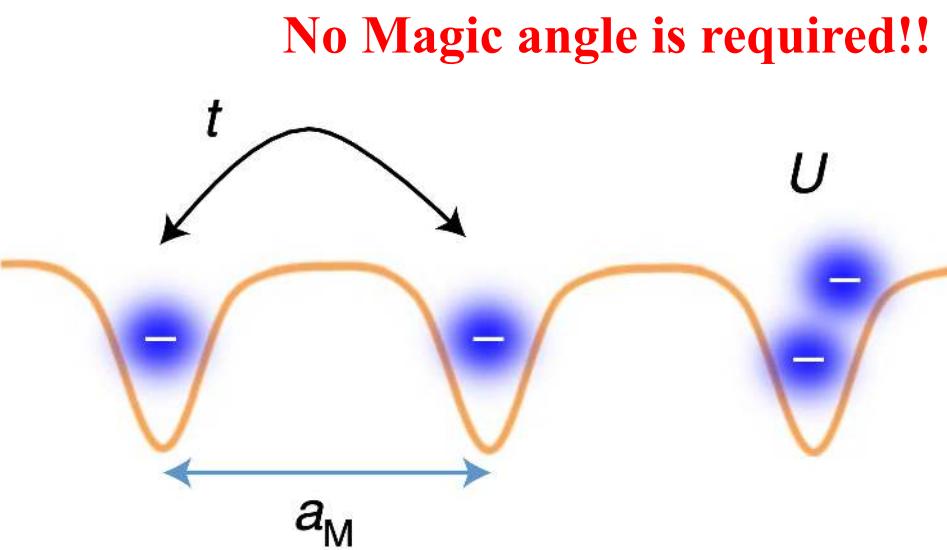
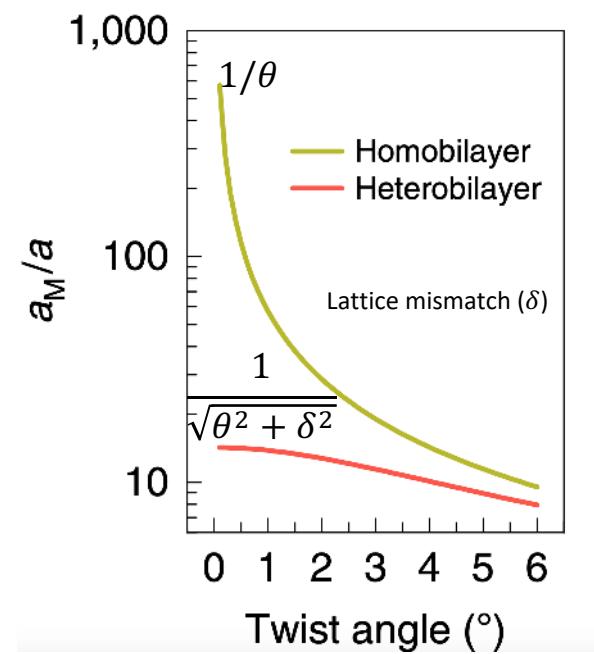
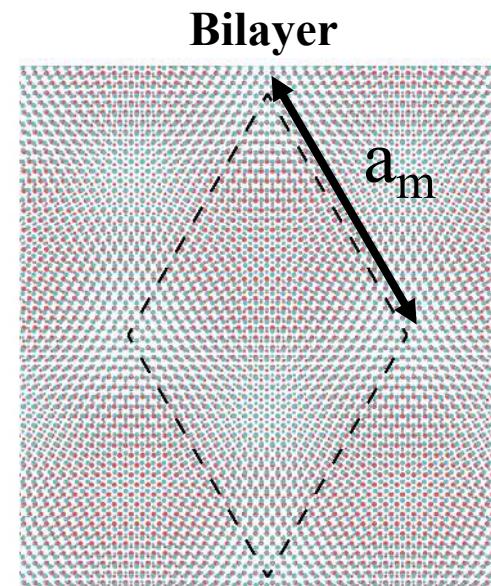


X. Xu, et al. Nature Phys. **10**, 343 (2014).
Di Xiao, et al. PRL **108**, 196802 (2012).

TMD (MX_2) moiré lattices



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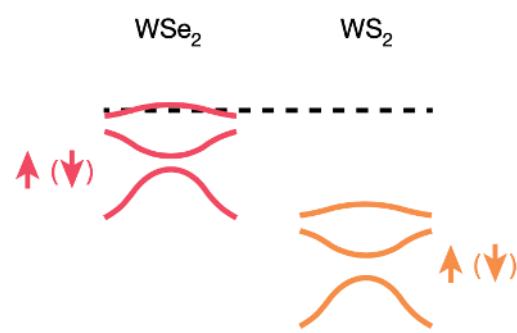
$$U \propto a_m^{-1/2}$$

$$t \propto a_m^{-2}$$

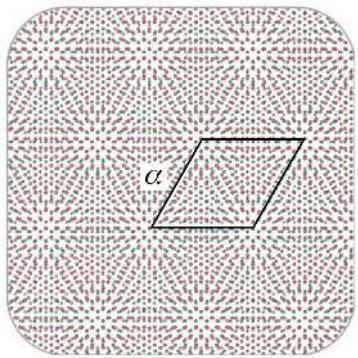
- K. F. Mak and J. Shan, Nature Nanotech. **17**, 686-695 (2022).
Y. Tang , et al. Nature **579**, 353-358 (2020).
E. C. Regan, et al. Nature **579**, 359-363 (2020).

TMD (MX_2) moiré lattices

Ex: $\text{WSe}_2\text{-WS}_2$ heterobilayer



Triangular moiré lattice

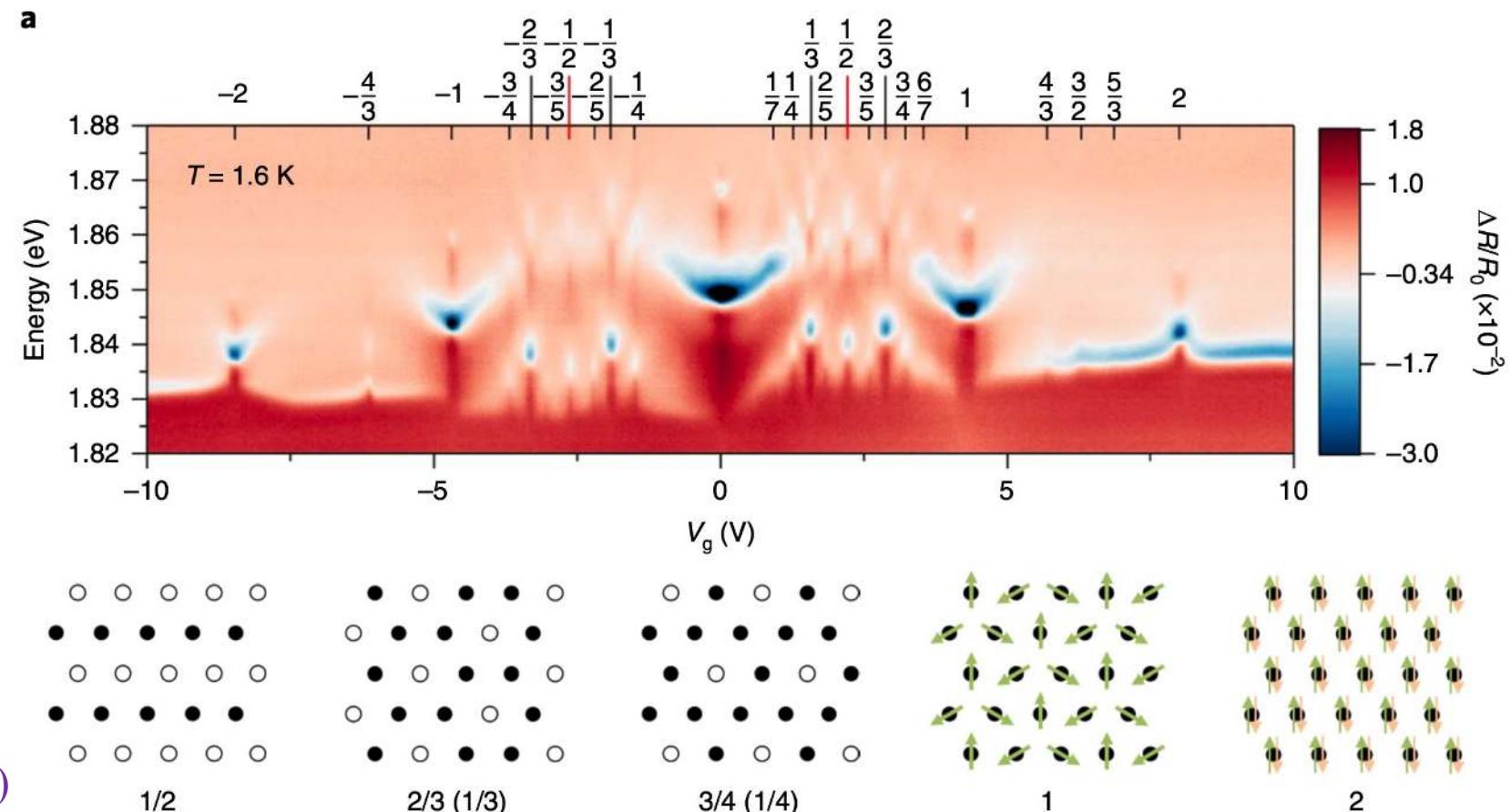


Y. Xu, et al. Nature **587**, 214–218 (2020)

C. Jin, et al. Nat. Mater. **20**, 940–944 (2021)

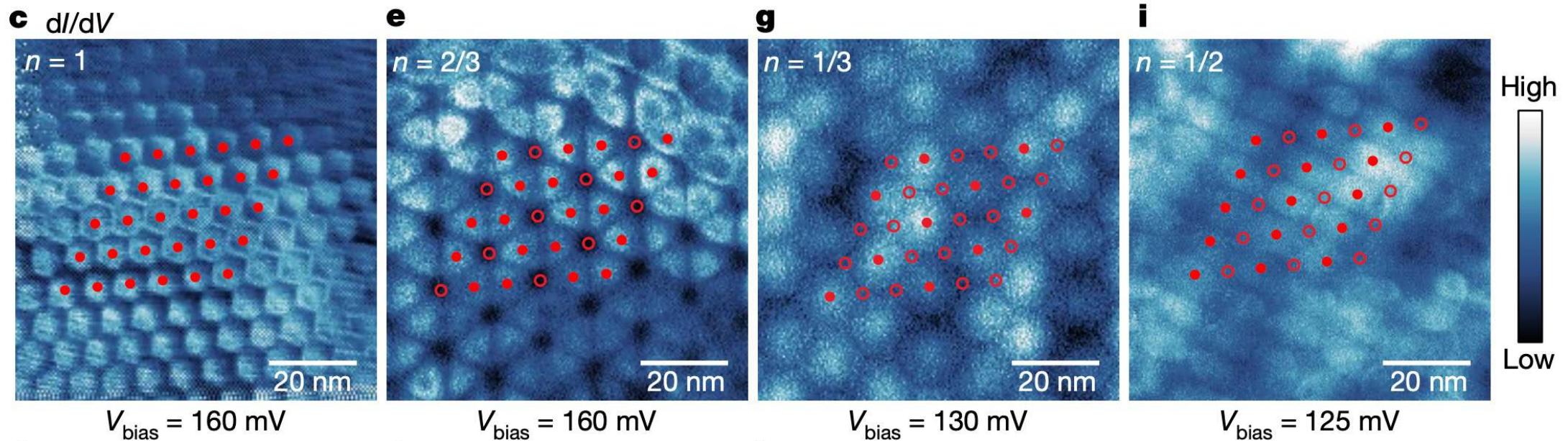
X. Huang, et al. Nature Phys. **17**, 715-719 (2021)

- Antiferromagnetic Mott state at half-filling ($n=1$).
- Multitude of Wigner Crystals at fractional fillings.



TMD (MX_2) moiré lattices

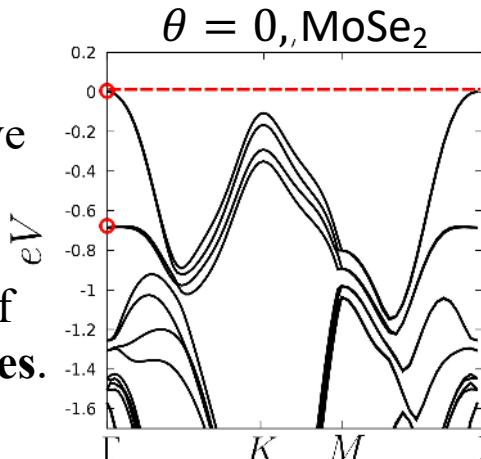
Real space images of Wigner crystals using STM



H. Li, et al. Nature **597**, 650-654 (2021).

Gamma-valley TMD's homobilayers:

- Ab-initio calculations suggests homo-bilayers of **MoSe₂**, **MoS₂**, and **WS₂** have **gamma-valley valence bands**.
- **Small twist angles** leads to formation of **Honeycomb and Kagome moiré lattices**.



M. Angeli and A. H. MacDonald, PNAS. USA **118**, e2021826118 (2021).

L. Xian, et al. Nat. Comm. **12**, 5644 (2021).

V. Vitale, et al. 2D Mater. **8**, 045010 (2021).

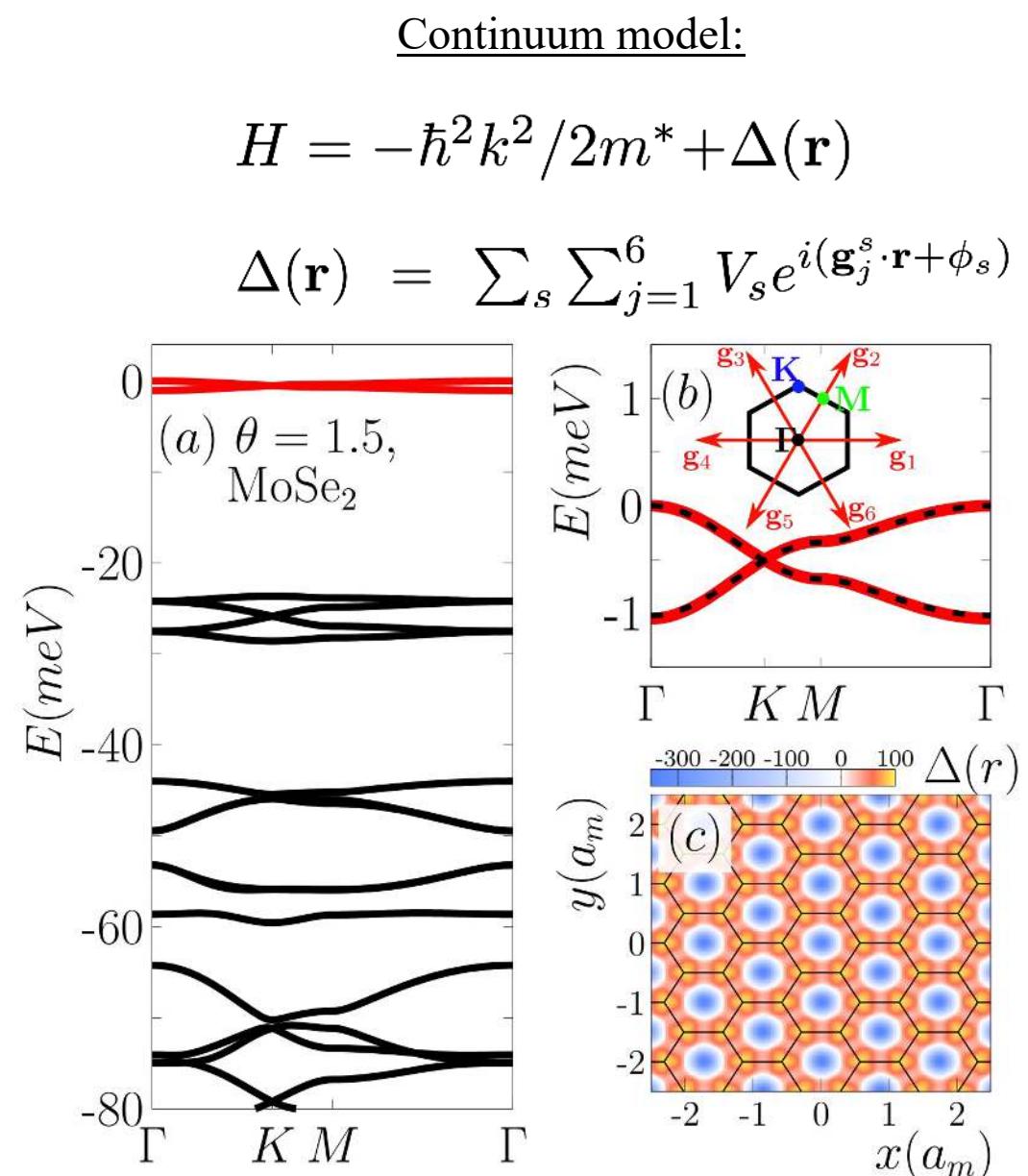
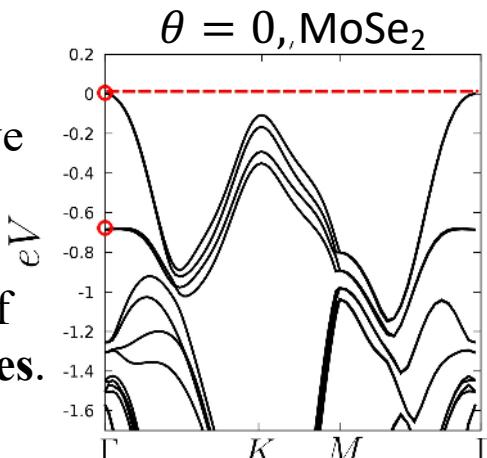
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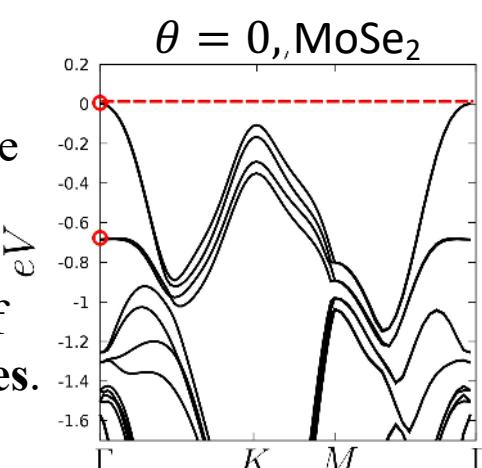
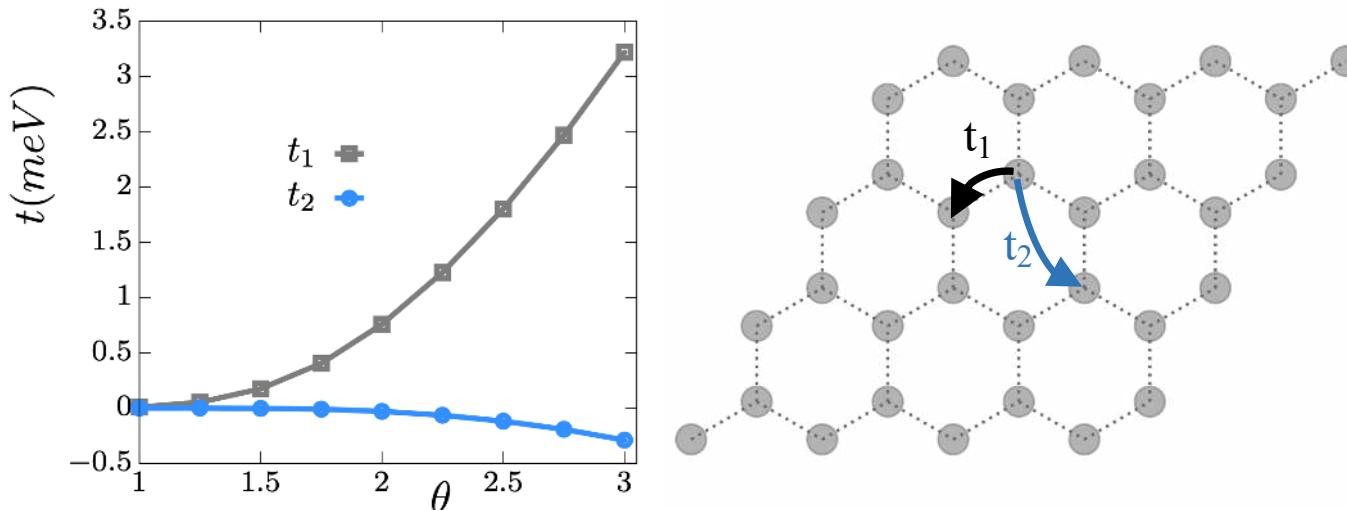
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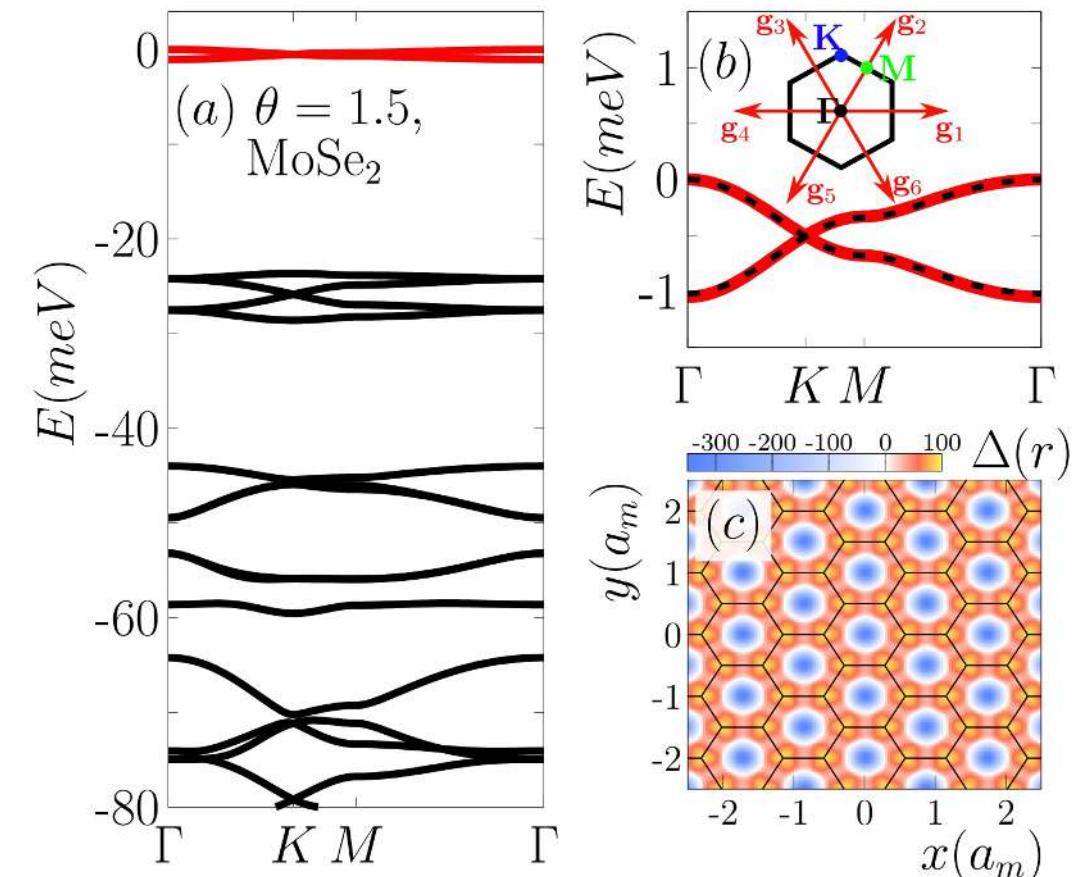
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 V. Vitale, et al. 2D Mater. **8**, 045010 (2021).



Continuum model:

$$H = -\hbar^2 k^2 / 2m^* + \Delta(\mathbf{r})$$

$$\Delta(\mathbf{r}) = \sum_s \sum_{j=1}^6 V_s e^{i(\mathbf{g}_j^s \cdot \mathbf{r} + \phi_s)}$$



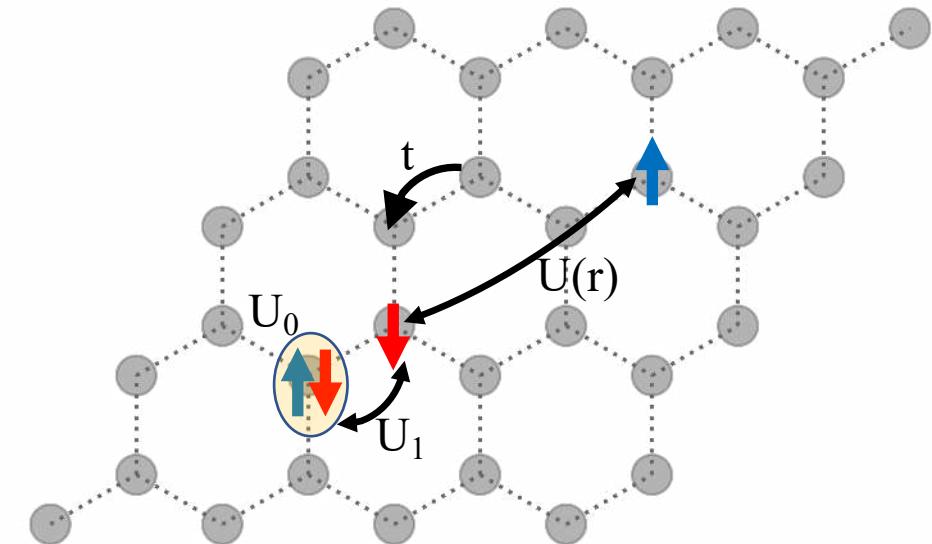
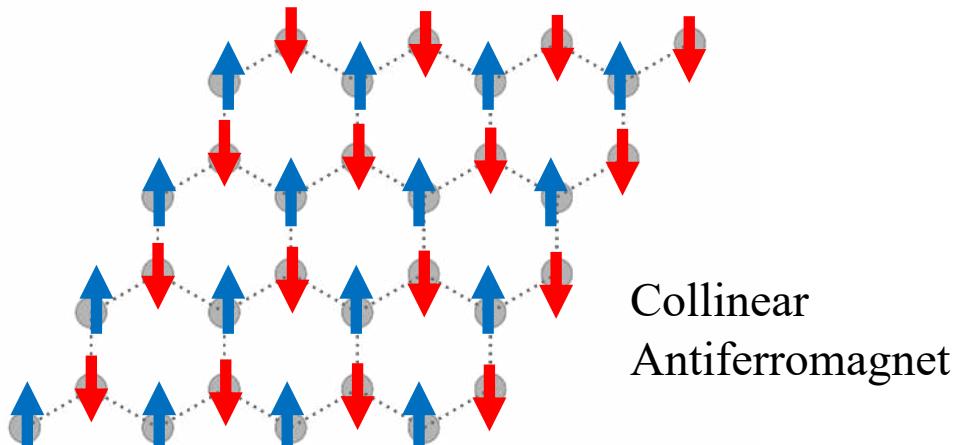
Model incorporating Coulomb repulsion:

$$H = \sum_{i,i',a,b,\sigma} t_{i'b}^{ia} c_{ia\sigma}^\dagger c_{i'b\sigma} + U_0 \sum_{i,a} n_{ia\uparrow} n_{ia\downarrow} \\ + U_1 \sum_i n_{i0} n_{i1} + 1/2 \sum_{i \neq i'} U_{ab}^{ii'} n_{ia} n_{i'b},$$

$$U(\mathbf{r}) = U_1 \left(\frac{1}{|\mathbf{r}|} - \frac{1}{\sqrt{|\mathbf{r}|^2 + d^2}} \right) / \left(\frac{1}{|\mathbf{r}_1|} - \frac{1}{\sqrt{|\mathbf{r}_1|^2 + d^2}} \right)$$

d is screening length

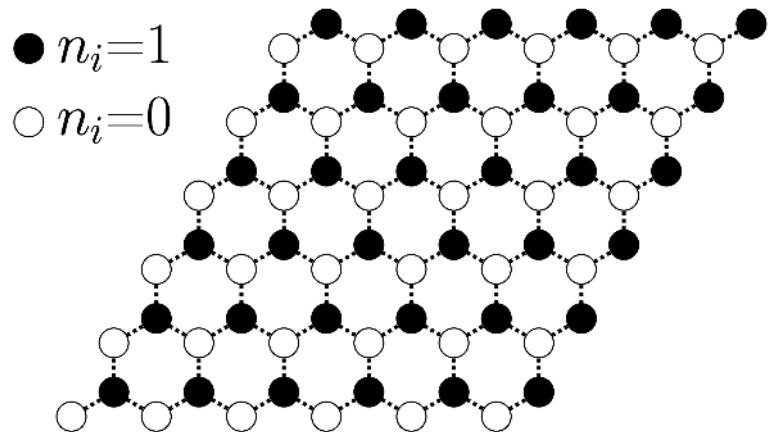
$n=1$ (half-filling)



Wigner Crystals at fractional fillings?

Wigner crystals at fractional fillings:

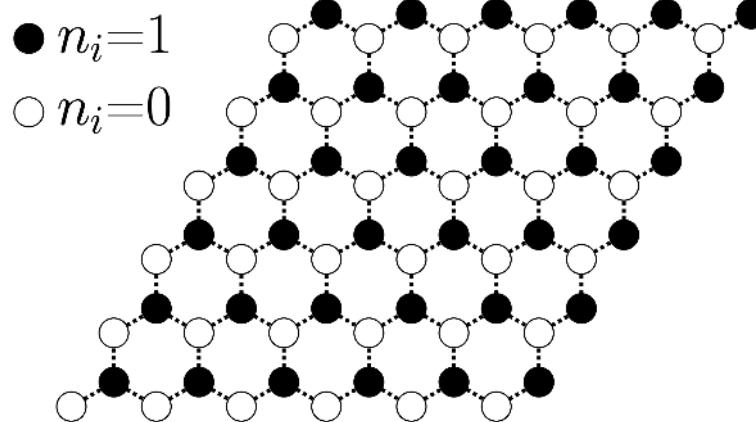
(a) $n = 1/2$, Triangular WC



- Emergent triangular Wigner crystal lattice.
- Possibility of having exotic magnetism in triangular lattices, including the quantum spin-liquids

Wigner crystals at fractional fillings:

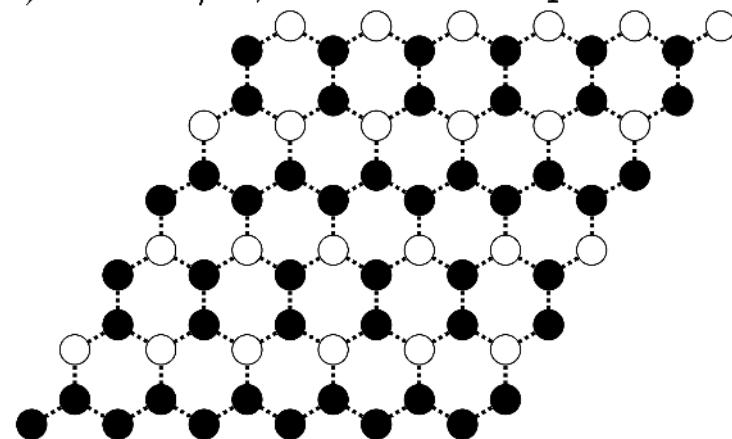
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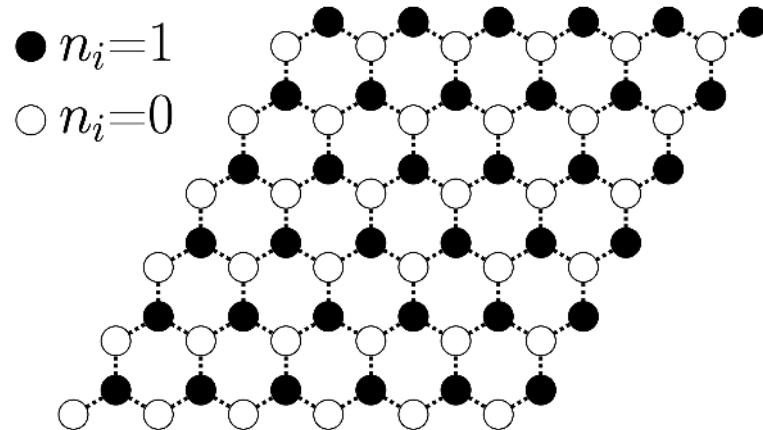
- Breaks rotational symmetry.
- Two kind of stripes formation.
- Quasi-1D geometries

(b) $n = 2/3$, Double-striped WC



Wigner crystals at fractional fillings:

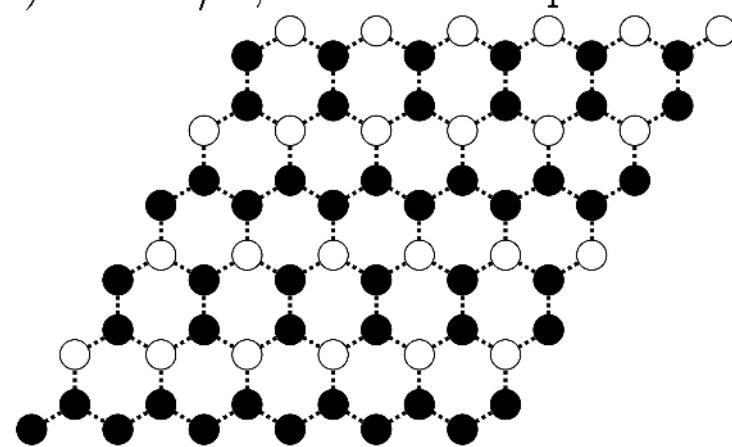
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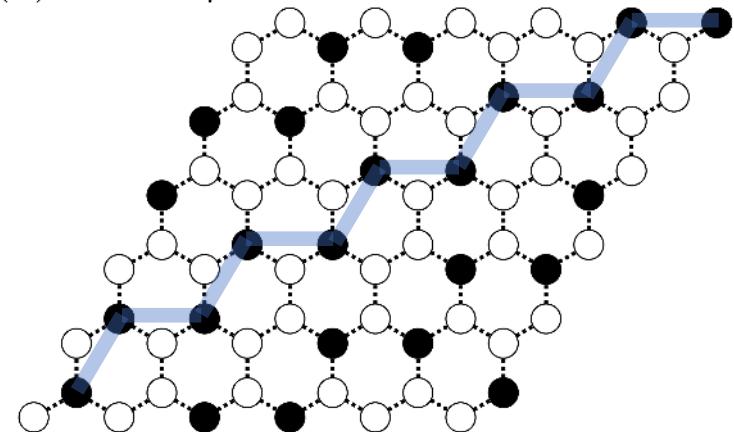
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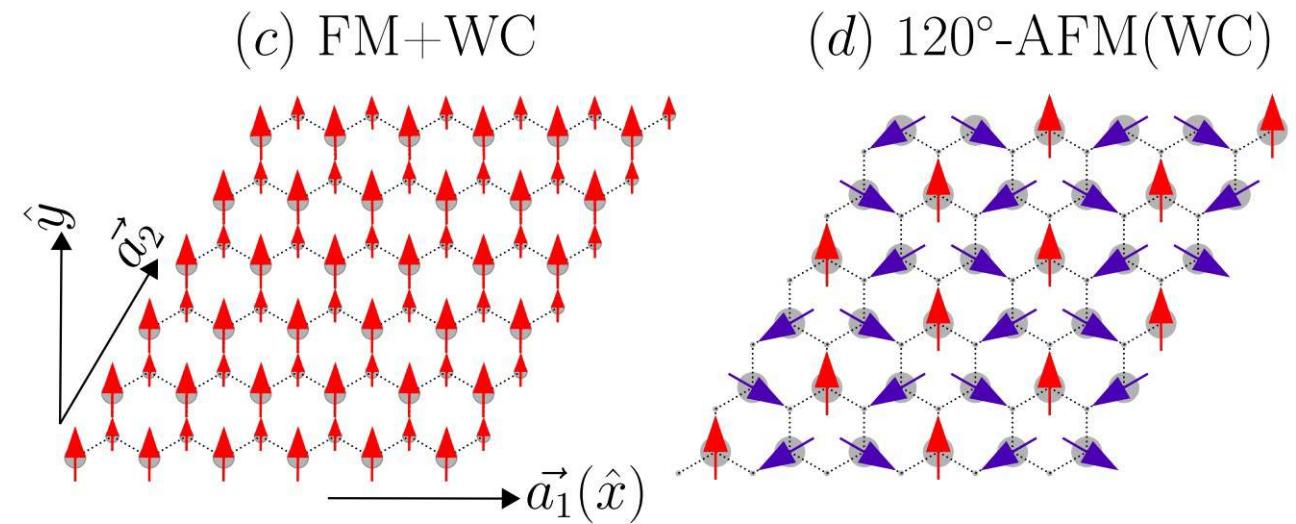
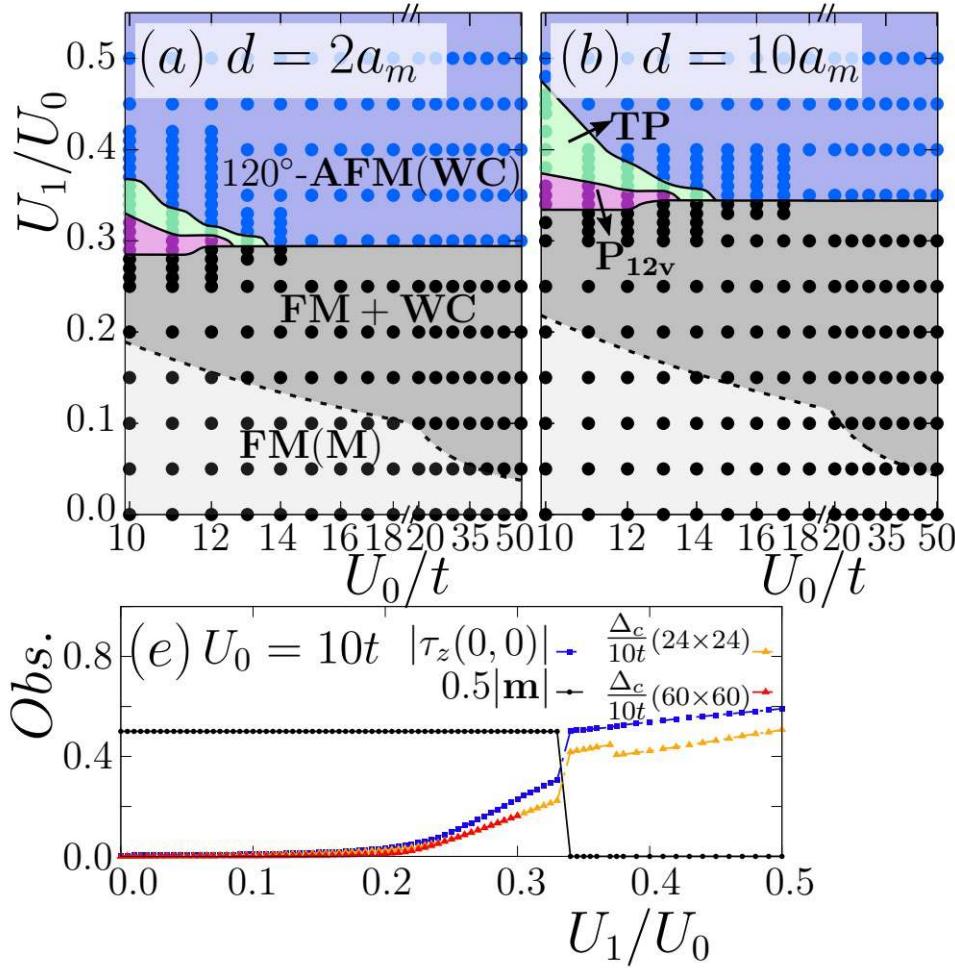


(c) $n = 1/3$, ZigZag WC

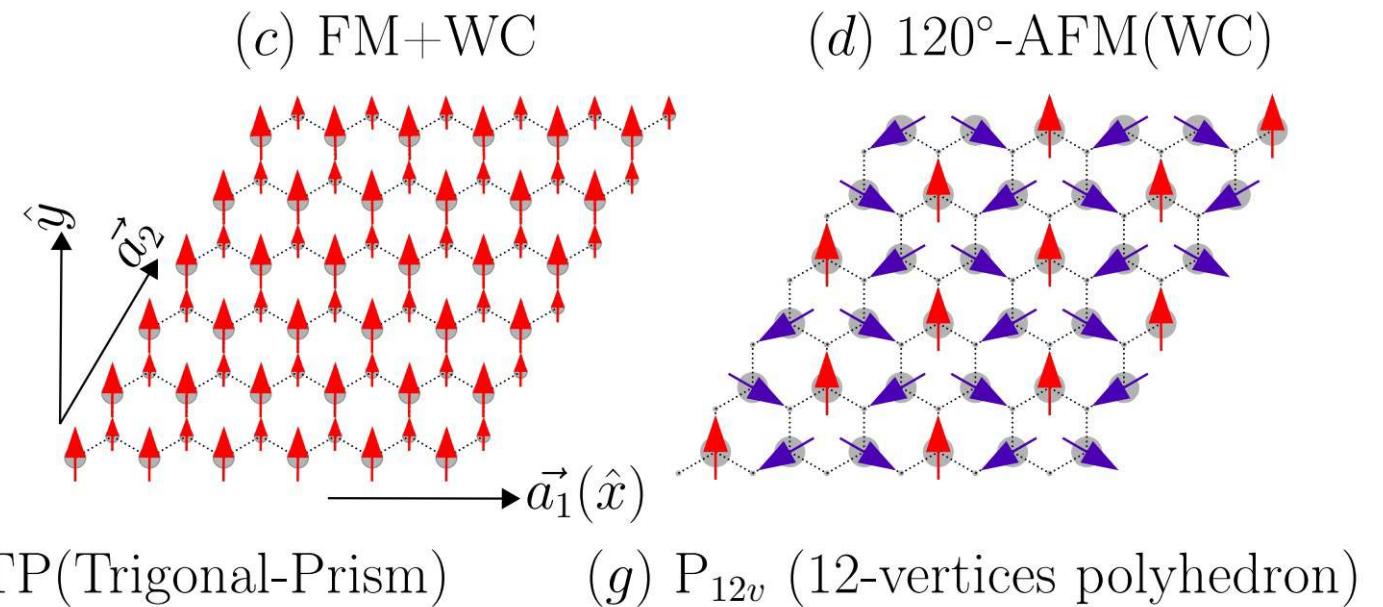
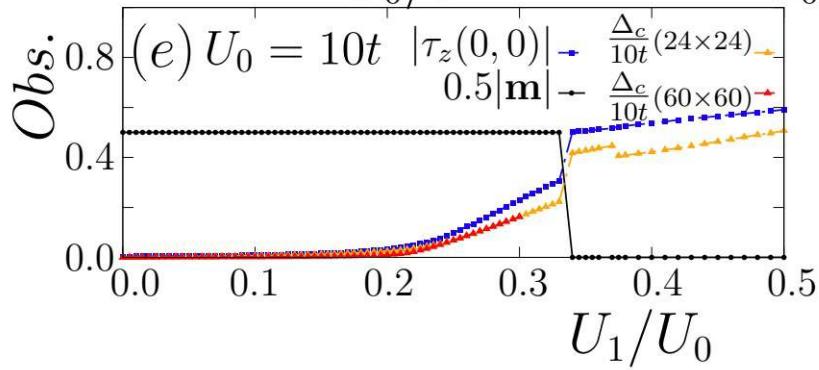
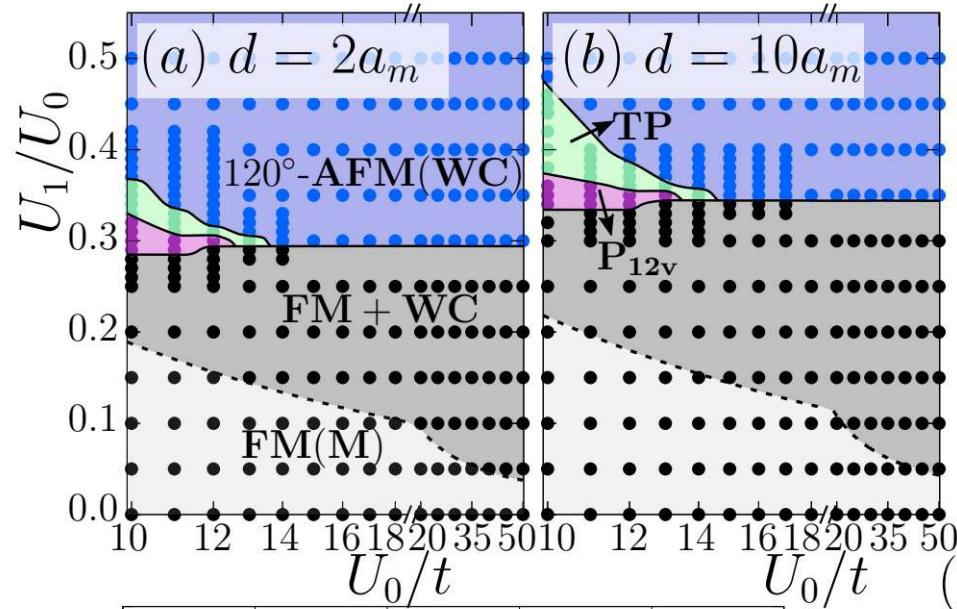


- Breaks rotational symmetry.
- Zigzag quasi-1D chains.

Results for n=1/2

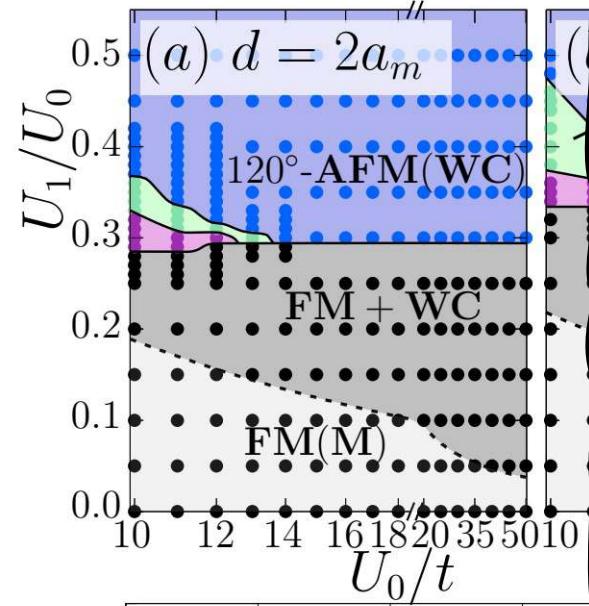


Results for n=1/2

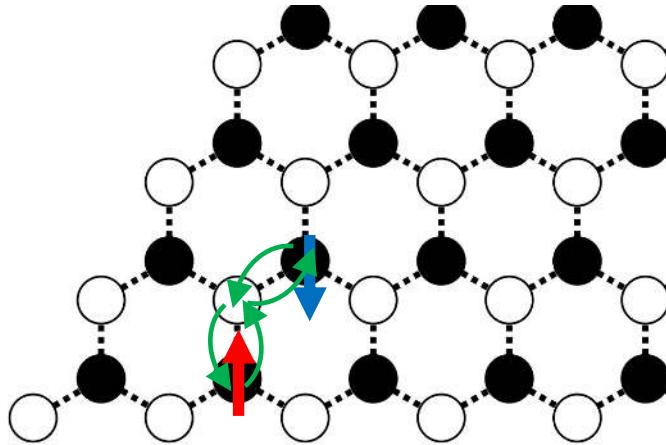


TP breaks
rotational
symmetry!!

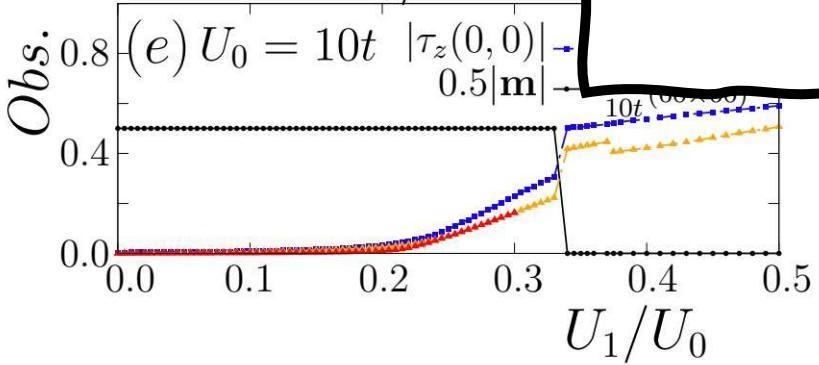
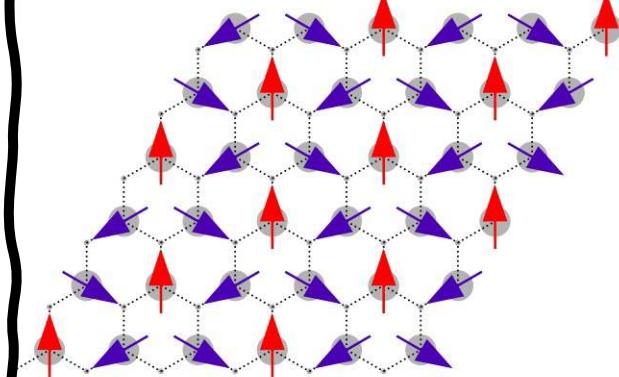
Results for $n=1/2$



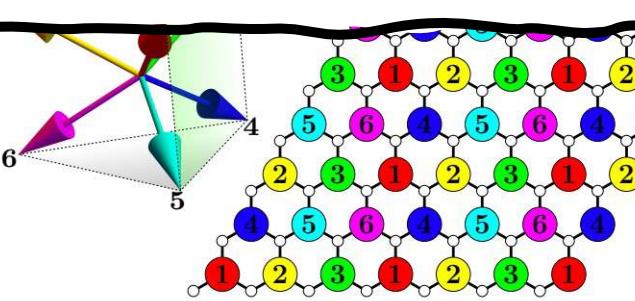
$$J \propto \frac{t^4}{(2U_1)^2 U_0}$$



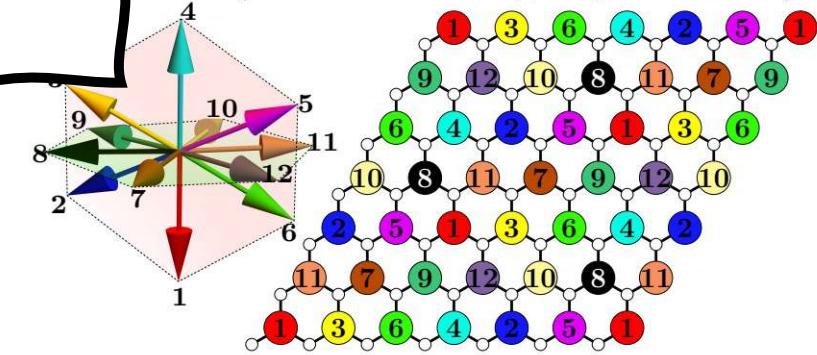
(d) 120°-AFM(WC)



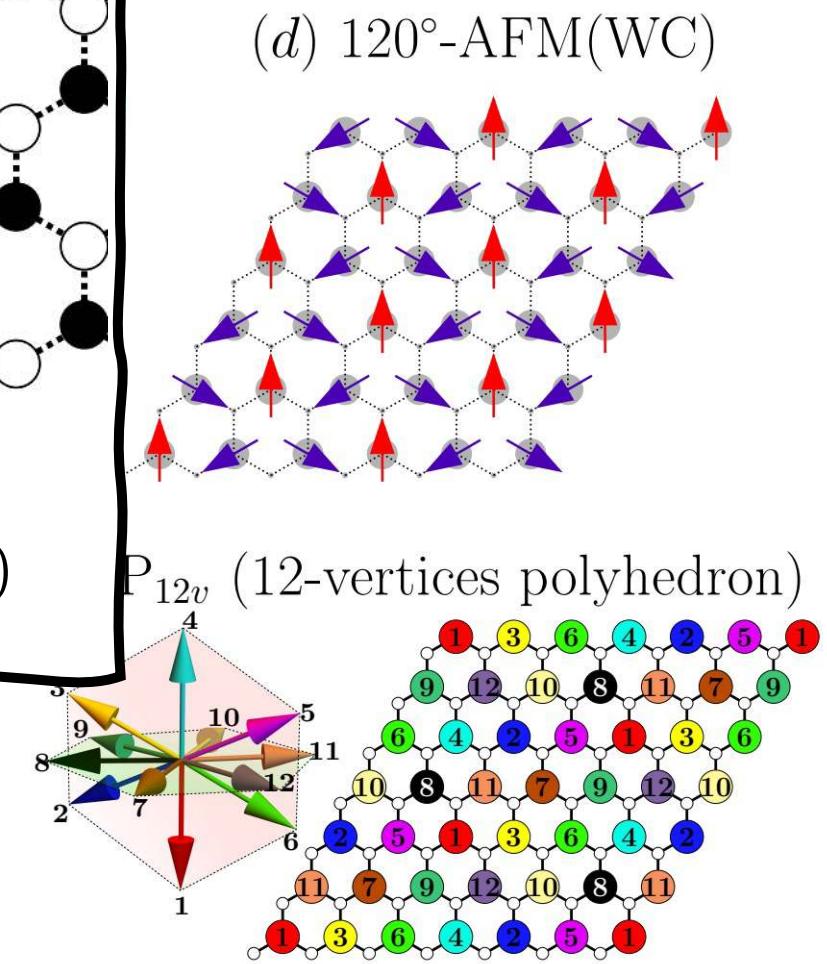
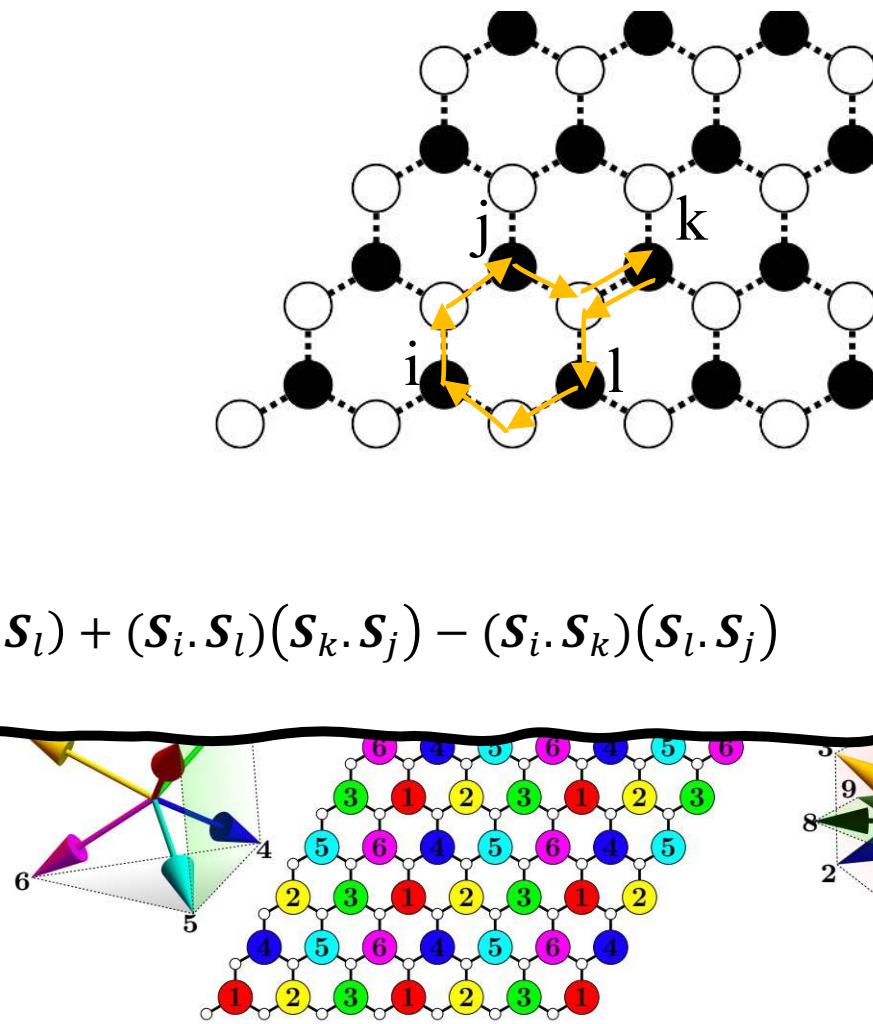
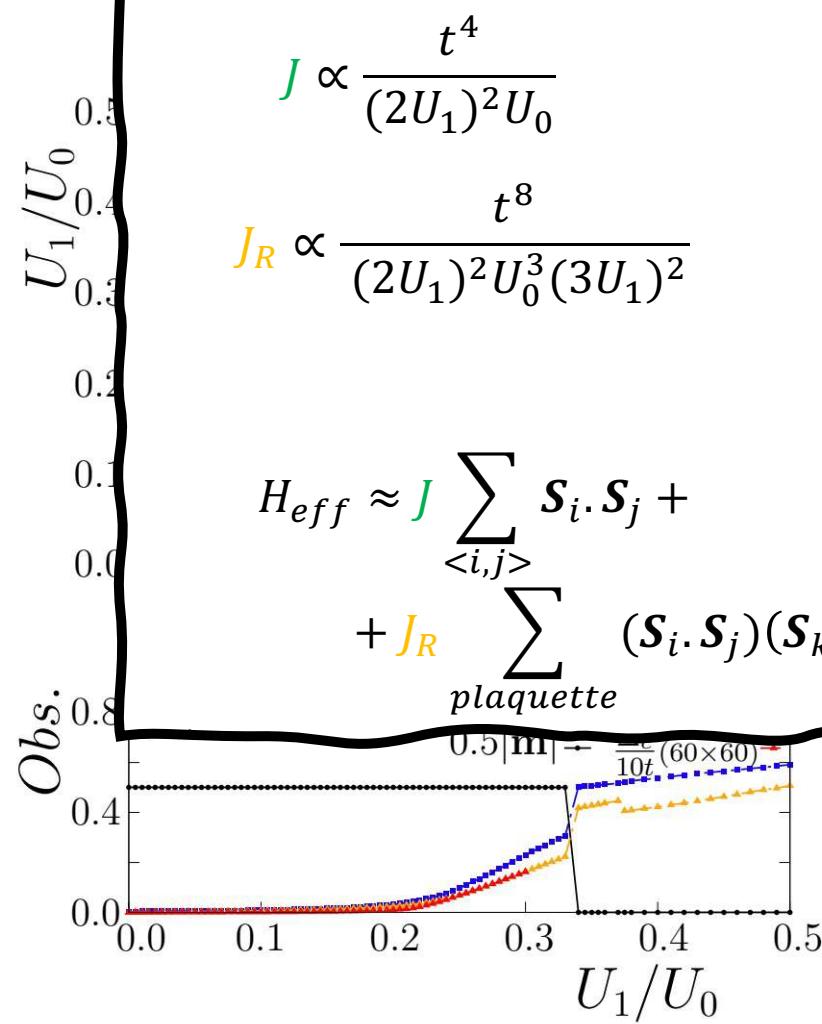
$$H_{eff} \approx J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$



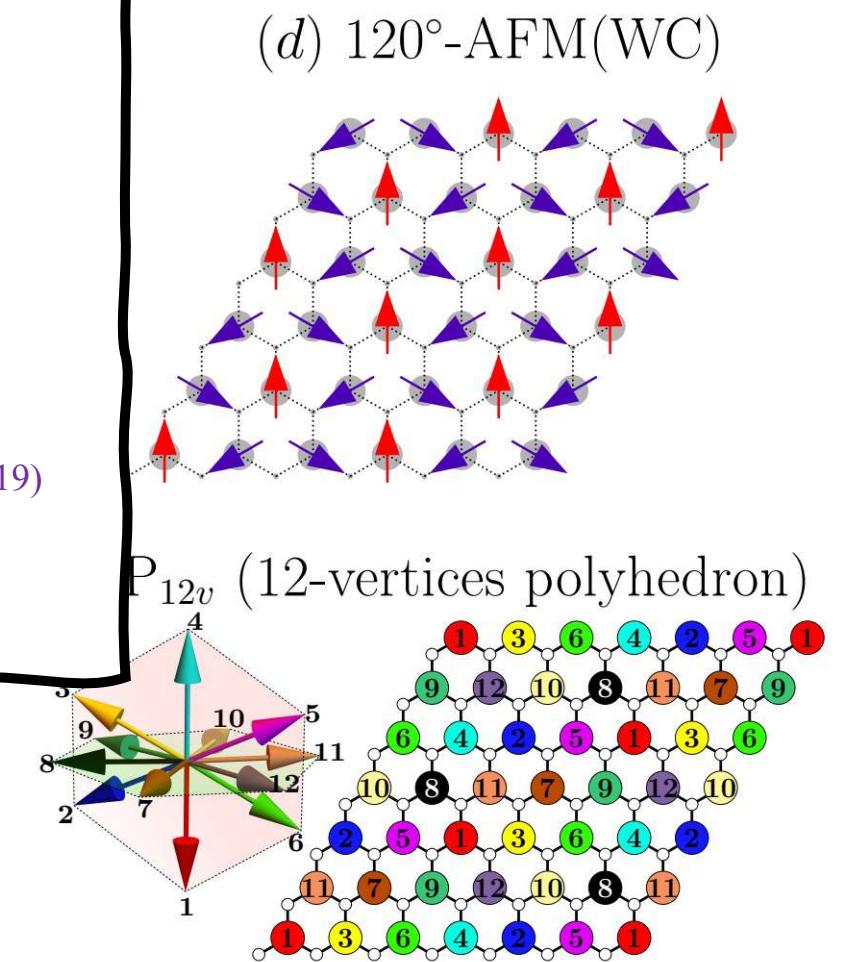
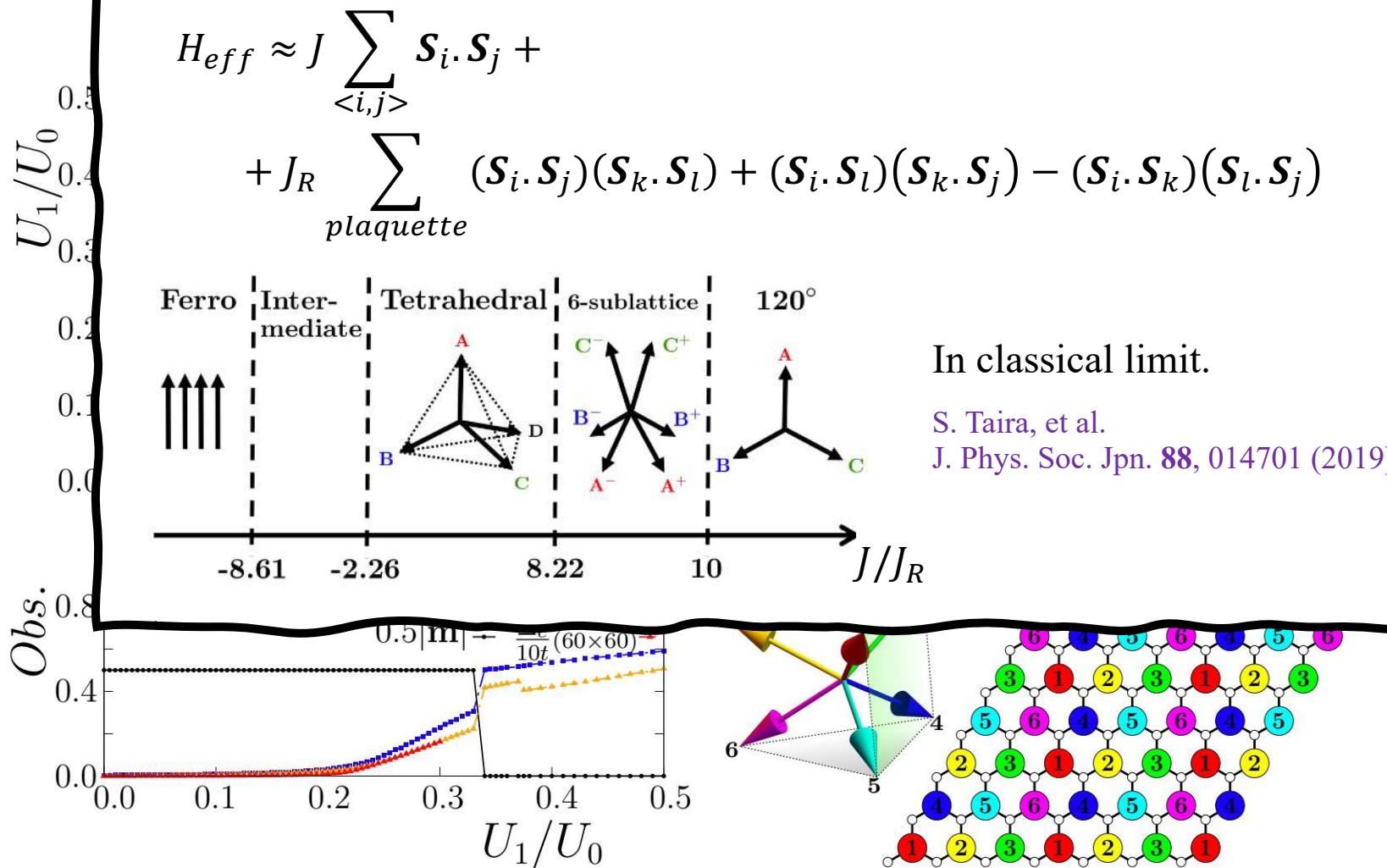
P_{12v} (12-vertices polyhedron)



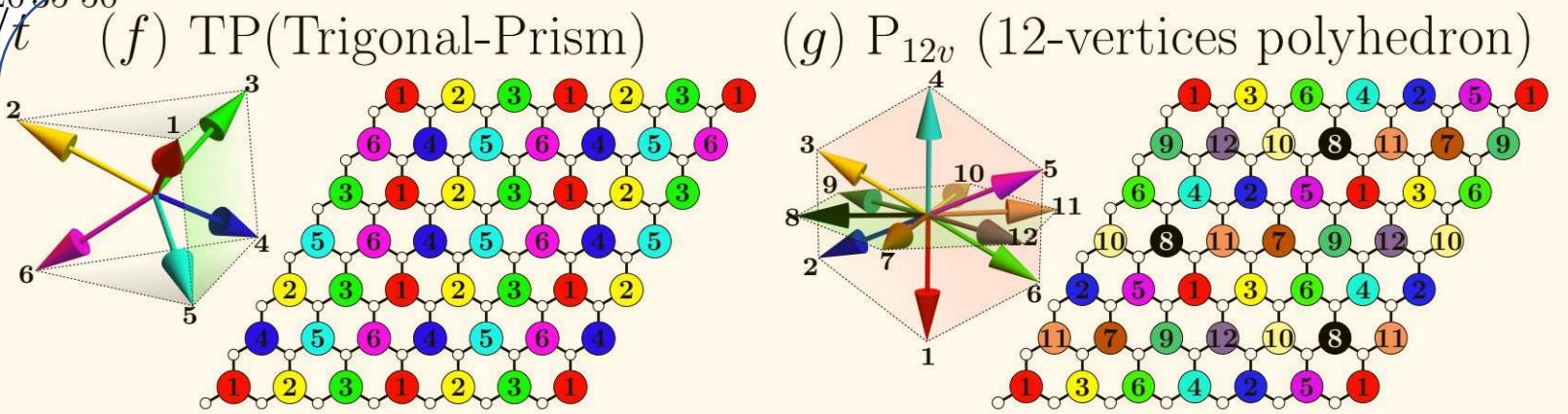
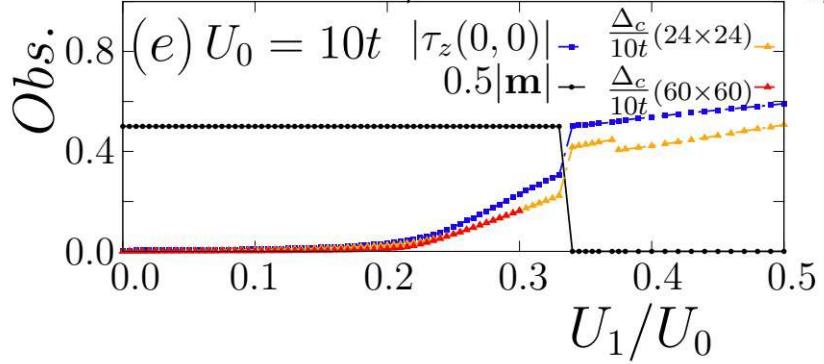
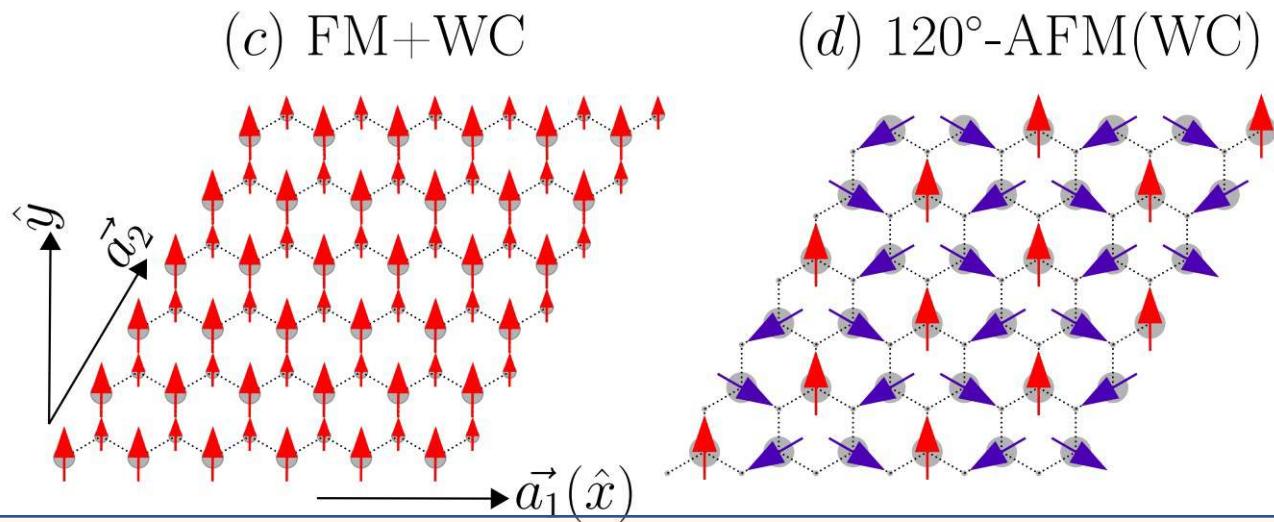
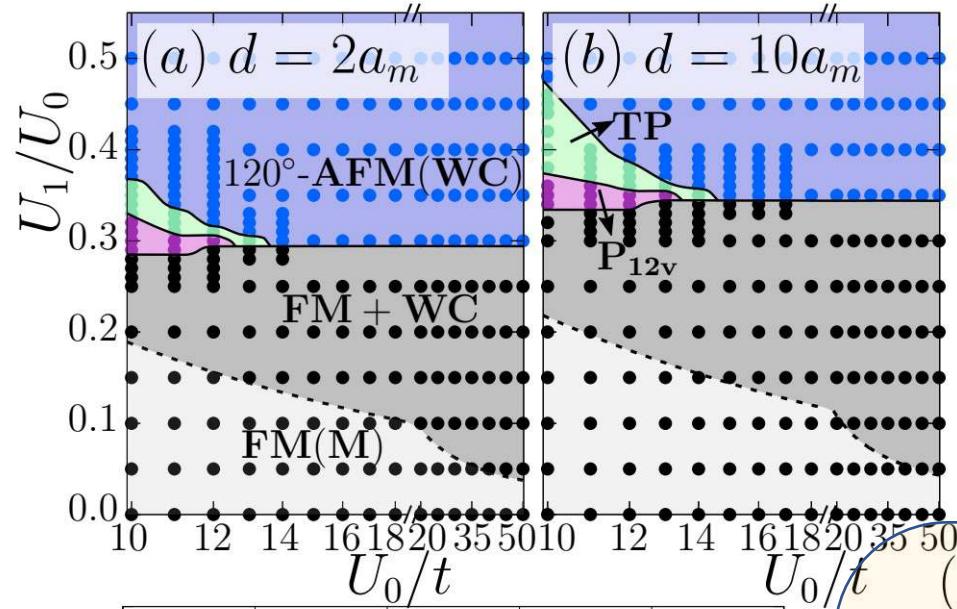
Results for $n=1/2$



Results for $n=1/2$

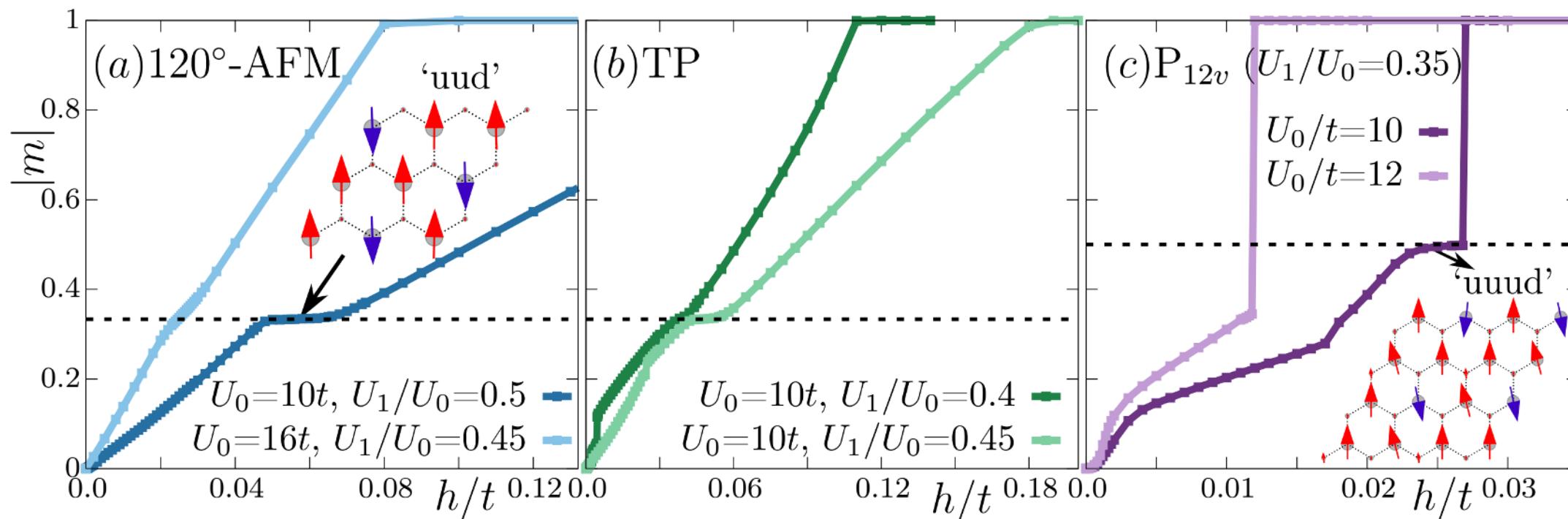


Results for $n=1/2$



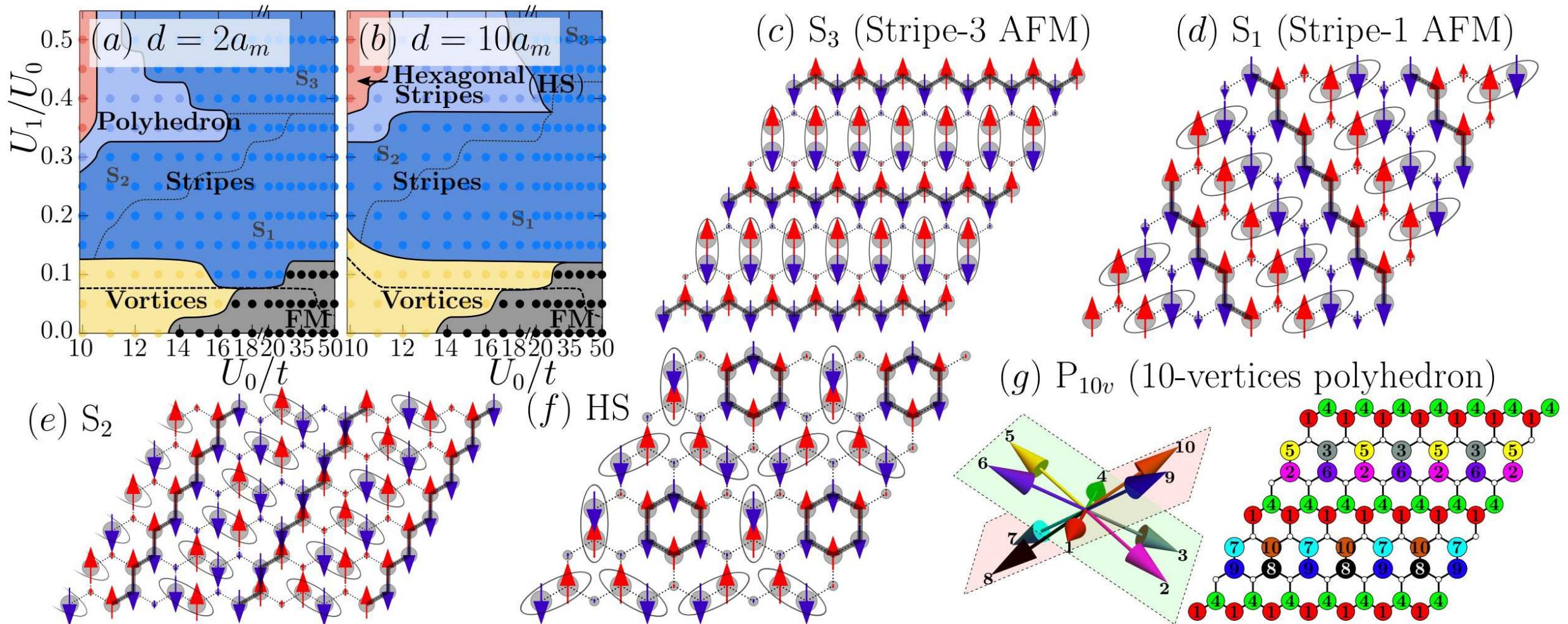
Quantum fluctuations can lead to
novel **quantum spin liquids!!**

Results for n=1/2 (Magnetization vs external field)

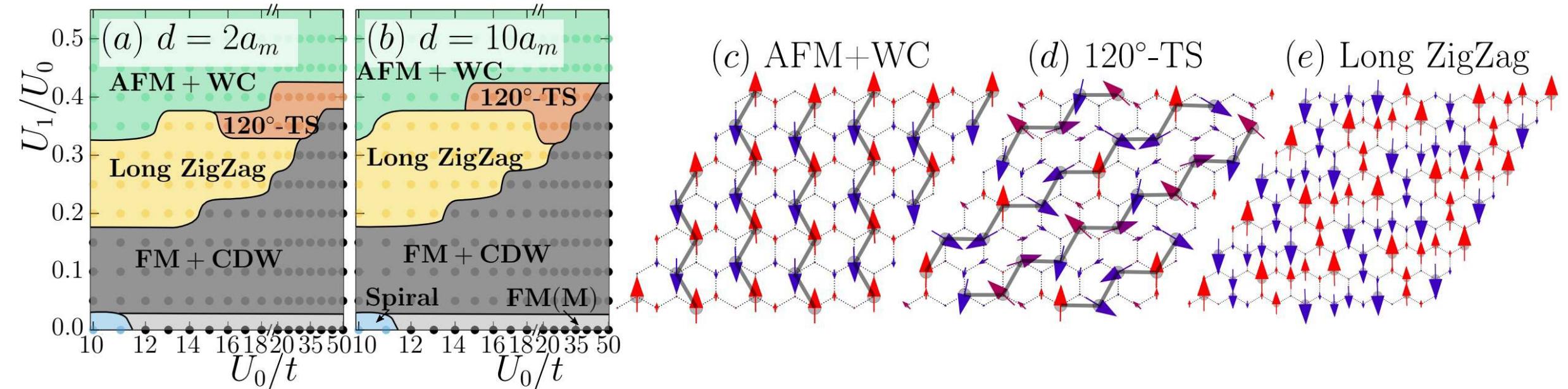


- $m=1/3$ plateaus in 120° -AFM and Trigonal prism state.
- $m=1/2$ plateau in P_{12v} state, followed by first order phase transition to saturated ferromagnet.

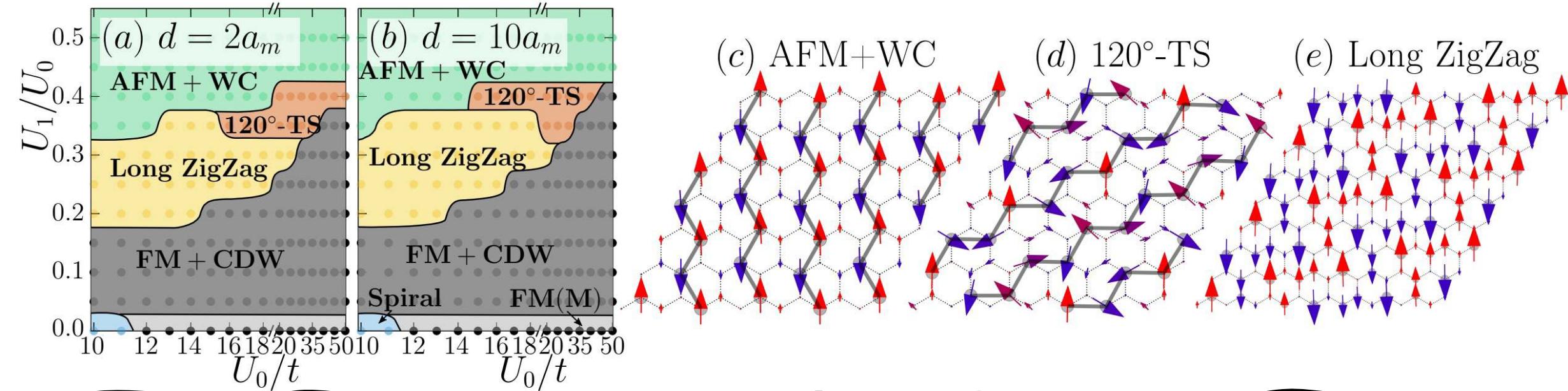
Results for $n=2/3$



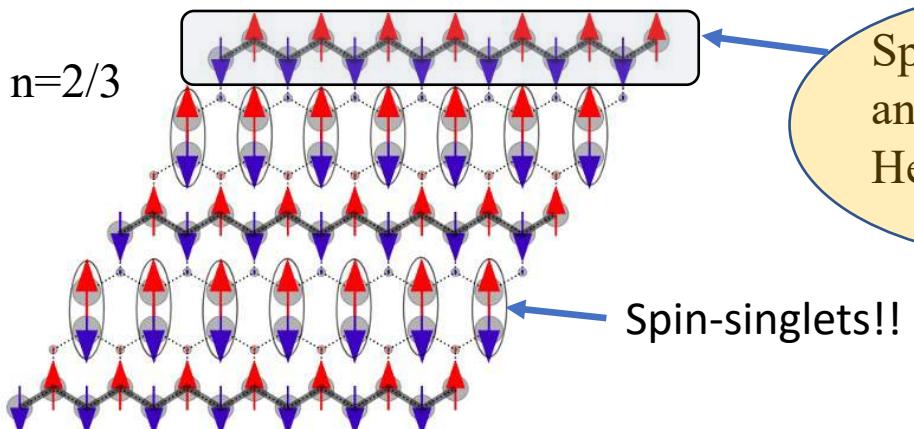
Results for $n=1/3$



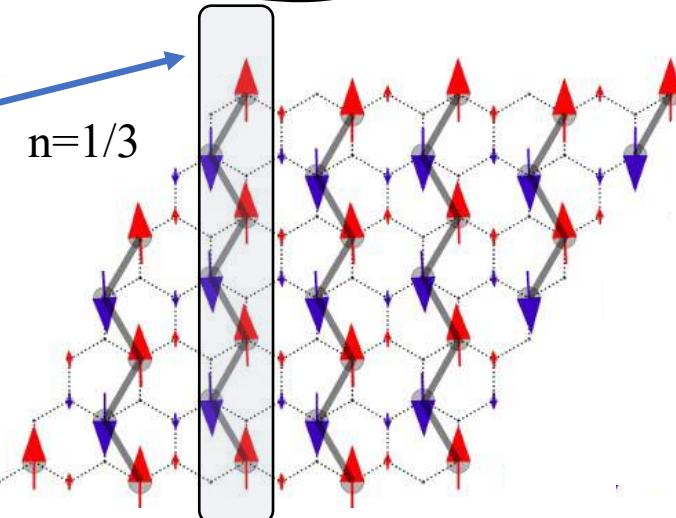
Results for $n=1/3$



Expected effect of quantum fluctuations on Wigner crystal magnetism:



Spin=1/2
antiferromagnetic
Heisenberg chains!!



Conclusions:

- Honeycomb moiré lattices can be realized in gamma-valley TMD homobilayers.
- Possibility for various Wigner crystals at fractionally filled moiré bands.
- Exotic magnetism including non-coplanar states and quasi-1D systems.
- Avenue for variety of quantum spin liquids.

Conclusions:

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 - Possibility for various Wigner crystals at fractionally filled moiré bands.
 - Exotic magnetism including non-coplanar states and quasi-1D systems.
 - Avenue for variety of quantum spin liquids.
-
- Hopefully experimentalists will synthesize gamma-valley TMD homobilayers.
 - Further theoretical investigations are required to explore the presence of possible quantum spin liquids.

Thanks!!

Extra slides

Few details on TBG:

- Monolayer $a=0.24\text{nm}$

Guohong Li, Rutgers (2009): STM Van Hove singularities observation

- amoire/ $a=32$, $\theta=1.79$
- amoire/ $a=50$, $\theta=1.16$

Bistritzer, MacDonald(2011):

Set of magic angles: 1.05, 0.5, 0.35, 0.24, 0.2

Y.Cao (2018) TBG:

Half-filling charge gap = 0.3meV i.e. thermal activation gap

Near $\theta=1$, bandwidth is near 10meV

