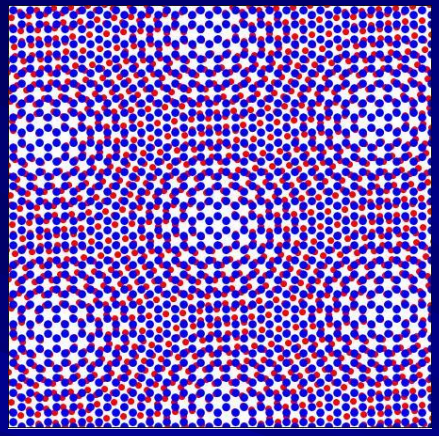
TIME-REVERSAL SYMMETRY BREAKING vs SPIN-POLARIZED PHASE FROM SCREENING OF COULOMB INTERACTION IN TWISTED BILAYER GRAPHENE



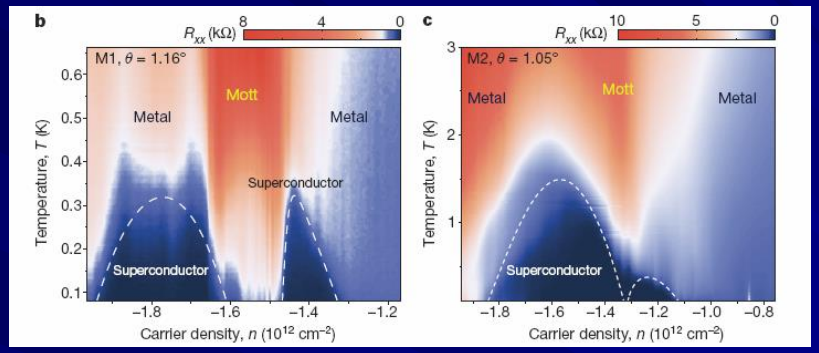
J. González[1] and T. Stauber[2]

[1]Instituto de Estructura de la Materia, CSIC, Spain

[2]Instituto de Ciencia de Materiales de Madrid, CSIC, Spain

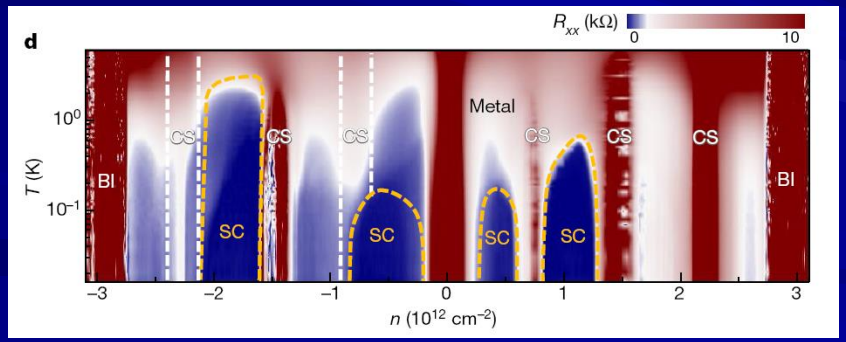
TWISTED BILAYER GRAPHENE

Magic-angle twisted bilayer graphene is a system with a very reach phase diagram, reflecting strong correlations at integer fillings



Y. Cao, V. Fatemi, S. Fang, K. Watanabe, T. Taniguchi, E. Kaxiras, and P. Jarillo-Herrero, Nature 556, 43 (2018)

Insulating states have been observed at integer fillings of the first valence and conduction bands



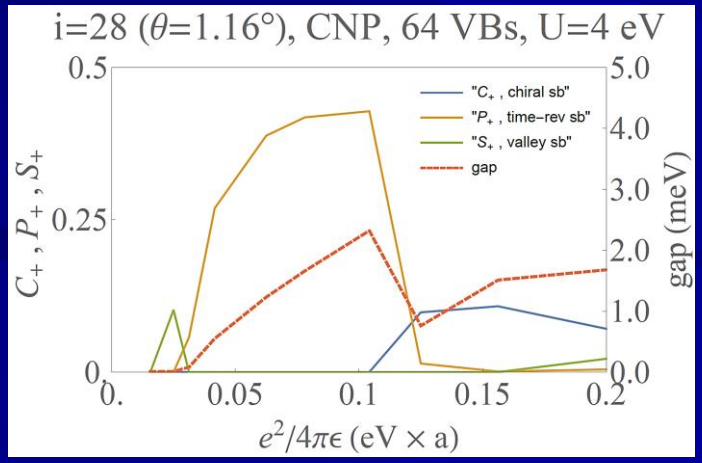
X. Lu *et al.*, Nature 574, 653 (2019)

TIME-REVERSAL SYMMETRY BREAKING VS SPIN-POLARIZED PHASE

There have been many studies of symmetry broken phases in twisted bilayer graphene

- Luis A. González-Arraga, J. L. Lado, F. Guinea, and P. San-José, Phys. Rev. Lett. 119, 107201 (2017).
- Y. Xie, *et al.*, Nature 572, 101 (2019).
- Y. Choi *et al.*, Nature Phys. 15, 1174 (2019).
- M. Xie and A. H. MacDonald, Phys. Rev. Lett. 124, 097601 (2020).
- J. Kang and O. Vafek, Phys. Rev. Lett. 122, 246401 (2019).
- T. Cea, N. R. Walet, and F. Guinea, Phys. Rev. B 100, 205113 (2019).
- L. Rademaker, D. A. Abanin, and P. Mellado, Phys. Rev. B 100, 205114 (2019).
- S. Liu, E. Khalaf, J. Y. Lee, and A. Vishwanath, Phys. Rev. Research 3, 013033 (2021).
- J. Liu and X. Dai, Phys. Rev. B 103, 035427 (2021).
- Y. Zhang, K. Jiang, Z. Wang, and F. Zhang, Phys. Rev. B 102, 035136 (2020).
- J. Kang and O. Vafek, Phys. Rev. B 102, 035161 (2020).
- T. Cea and F. Guinea, Phys. Rev. B 102, 045107 (2020).
- X. Lin and J. Ni, Phys. Rev. B 102, 035441 (2020).
- T. Soejima, D. E. Parker, N. Bultinck, J. Hauschild, and M. P. Zaletel, Phys. Rev. B 102, 205111 (2020).
- J. González and T. Stauber, Phys. Rev. B 102, 081118 (2020).

At the charge neutrality point, there may be several phases arising from the breakdown of symmetry in the charge sector

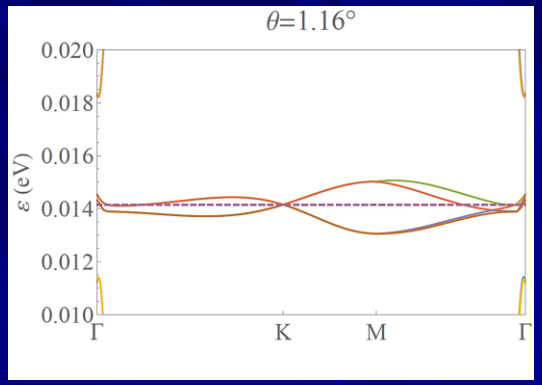


J. G. and T. Stauber,
PRB 102, 081118(R) (2020)

TIME-REVERSAL SYMMETRY BREAKING VS SPIN-POLARIZED PHASE

But one may also ask about the possibility of having magnetic instabilities for sufficiently strong on-site (Hubbard) repulsion.

We study the dynamical symmetry breaking by means of a self-consistent Hartree-Fock approximation in real space, starting from a tight-binding approach.



The noninteracting Hamiltonian H_0 can be represented in the form

$$H_0 = -\sum_{\langle i,j\rangle} t_{\parallel}(\mathbf{r}_i - \mathbf{r}_j)\,(a^{+}_{1,i}a_{1,j} + h.c.) - \sum_{\langle i,j\rangle} t_{\parallel}(\mathbf{r}_i - \mathbf{r}_j)\,(a^{+}_{2,i}a_{2,j} + h.c.) - \sum_{\langle i,j\rangle} t_{\perp}(\mathbf{r}_i - \mathbf{r}_j)\,(a^{+}_{1,i}a_{2,j} + h.c.)$$

The interacting part of the Hamiltonian H_{int} has in general two different contributions

$$H_{\text{int}} = H_C + H_U$$

$$H_C = \frac{1}{2}\sum_{i,j,\sigma,\sigma'} a^{+}_{i\sigma}a_{i\sigma}\; v_C(\mathbf{r}_i - \mathbf{r}_j)\; a^{+}_{j\sigma'}a_{j\sigma'} \qquad v_C(\mathbf{r}) = \frac{e^2}{4\pi\varepsilon} 2\sqrt{2}\,\frac{e^{-\pi r/\xi}}{\xi\sqrt{r/\xi}}$$

$$H_U = U\sum_i a^{+}_{i\uparrow}a_{i\uparrow}\; a^{+}_{i\downarrow}a_{i\downarrow}$$

TIME-REVERSAL SYMMETRY BREAKING VS SPIN-POLARIZED PHASE

The noninteracting Hamiltonian H_0 admits in general a matrix representation in terms of its eigenvalues and eigenvectors

$$\left(H_0\right)_{i\sigma,j\sigma} = \sum_a \varepsilon^0_{a\sigma}\, \phi^0_{a\sigma}(\mathbf{r}_i)\, \phi^0_{a\sigma}(\mathbf{r}_j)^*$$

The noninteracting electron propagator G_0 becomes in the zero-frequency (static) limit

$$\left(G_0\right)_{i\sigma,j\sigma} = -\sum_a \frac{1}{\varepsilon^0_{a\sigma}}\, \phi^0_{a\sigma}(\mathbf{r}_i)\, \phi^0_{a\sigma}(\mathbf{r}_j)^*$$

The Hartree-Fock approximation proceeds by assuming that the full electron propagator G has a similar representation

$$\left(G\right)_{i\sigma,j\sigma} = -\sum_a \frac{1}{\varepsilon_{a\sigma}}\, \phi_{a\sigma}(\mathbf{r}_i)\, \phi_{a\sigma}(\mathbf{r}_j)^*$$

The diagrammatics dictates the expression of the self-energy Σ in the equation

$$G^{-1} = G_0^{-1} - \Sigma$$

which is given by

$$\left(\Sigma\right)_{i\sigma,j\sigma} = 2\,\mathbf{1}_{ij} \sum_{\substack{\text{filled}\\ \text{bands}}} \sum_{l\sigma'} v_{\sigma\sigma'}(\mathbf{r}_i - \mathbf{r}_l)\, \left|\phi_{a\sigma'}(\mathbf{r}_l)\right|^2$$

$$- v_{\sigma\sigma}(\mathbf{r}_i - \mathbf{r}_j) \sum_{\substack{\text{filled}\\ \text{bands}}} \phi_{a\sigma}(\mathbf{r}_i)\, \phi_{a\sigma}(\mathbf{r}_j)^*$$

TIME-REVERSAL SYMMETRY BREAKING VS SPIN-POLARIZED PHASE

The condensation of different order parameters can be studied through the matrix elements

$$h_{ij}^{(\sigma)} = \sum_{\substack{\text{filled} \\ \text{bands}}} \phi_{a\sigma}(\mathbf{r}_i)\,\phi_{a\sigma}(\mathbf{r}_j)^*$$

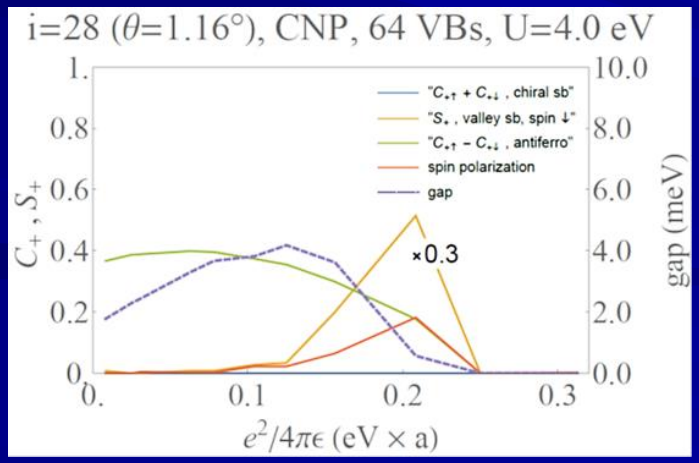
Chiral symmetry breaking and antiferromagnetic order can be characterized by the staggered order in sublattices A and B

$$C_{\pm\sigma} = \sum_{i\in A_1} h_{ii}^{(\sigma)} - \sum_{i\in B_1} h_{ii}^{(\sigma)} \pm \left(\sum_{i\in A_2} h_{ii}^{(\sigma)} - \sum_{i\in B_2} h_{ii}^{(\sigma)} \right)$$

and time-reversal symmetry breaking, with currents along nearest neighbors i_1, i_2, i_3 of each site

$$S_{+\sigma} = \mathrm{Im}\left(\sum_{i\in A_1} (h_{i_1 i_2}^{(\sigma)} h_{i_2 i_3}^{(\sigma)} h_{i_3 i_1}^{(\sigma)})^{1/3} - \sum_{i\in B_1} (h_{i_1 i_2}^{(\sigma)} h_{i_2 i_3}^{(\sigma)} h_{i_3 i_1}^{(\sigma)})^{1/3} + \sum_{i\in A_2} (h_{i_1 i_2}^{(\sigma)} h_{i_2 i_3}^{(\sigma)} h_{i_3 i_1}^{(\sigma)})^{1/3} - \sum_{i\in B_2} (h_{i_1 i_2}^{(\sigma)} h_{i_2 i_3}^{(\sigma)} h_{i_3 i_1}^{(\sigma)})^{1/3} \right)$$

charge neutrality point



$$v_C(\mathbf{r}) = \frac{e^2}{4\pi\varepsilon} 2\sqrt{2} \frac{e^{-\pi r/\xi}}{\xi\sqrt{r/\xi}}$$

$U = 4.0$ eV

J. G. and T. Stauber,
arXiv:2103.09015

TIME-REVERSAL SYMMETRY BREAKING VS SPIN-POLARIZED PHASE

The condensation of different order parameters can be studied through the matrix elements

$$h_{ij}^{(\sigma)} = \sum_{\substack{\text{filled} \\ \text{bands}}} \phi_{a\sigma}(\mathbf{r}_i)\,\phi_{a\sigma}(\mathbf{r}_j)^*$$

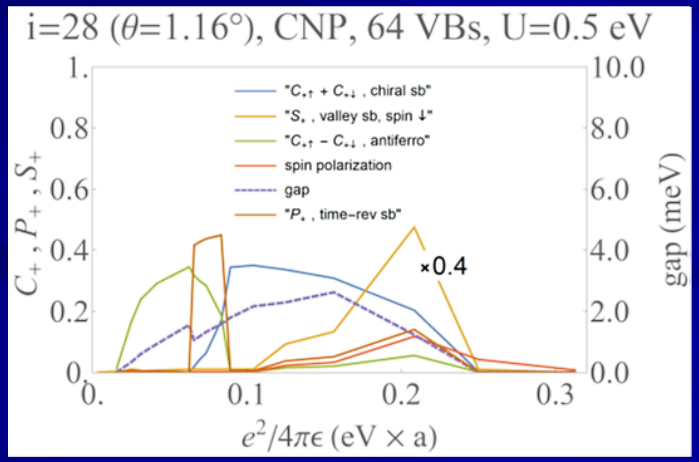
Chiral symmetry breaking and antiferromagnetic order can be characterized by the staggered order in sublattices A and B

$$C_{\pm\sigma} = \sum_{i\in A_1} h_{ii}^{(\sigma)} - \sum_{i\in B_1} h_{ii}^{(\sigma)} \pm \left(\sum_{i\in A_2} h_{ii}^{(\sigma)} - \sum_{i\in B_2} h_{ii}^{(\sigma)} \right)$$

and time-reversal symmetry breaking, with currents along nearest neighbors i_1, i_2, i_3 of each site

$$P_{+\sigma} = \mathrm{Im}\left(\sum_{i\in A_1} (h_{i_1 i_2}^{(\sigma)} h_{i_2 i_3}^{(\sigma)} h_{i_3 i_1}^{(\sigma)})^{1/3} + \sum_{i\in B_1} (h_{i_1 i_2}^{(\sigma)} h_{i_2 i_3}^{(\sigma)} h_{i_3 i_1}^{(\sigma)})^{1/3} + \sum_{i\in A_2} (h_{i_1 i_2}^{(\sigma)} h_{i_2 i_3}^{(\sigma)} h_{i_3 i_1}^{(\sigma)})^{1/3} + \sum_{i\in B_2} (h_{i_1 i_2}^{(\sigma)} h_{i_2 i_3}^{(\sigma)} h_{i_3 i_1}^{(\sigma)})^{1/3} \right)$$

charge neutrality point



$$v_C(\mathbf{r}) = \frac{e^2}{4\pi\varepsilon} 2\sqrt{2}\, \frac{e^{-\pi r/\xi}}{\xi\sqrt{r/\xi}}$$

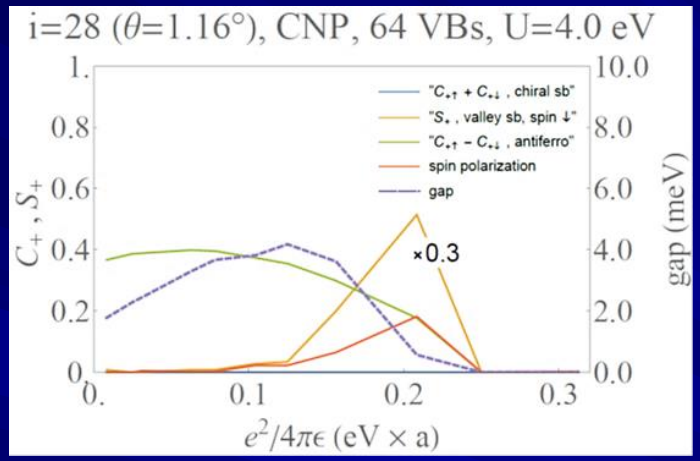
$U = 0.5$ eV

J. G. and T. Stauber,
arXiv:2103.09015

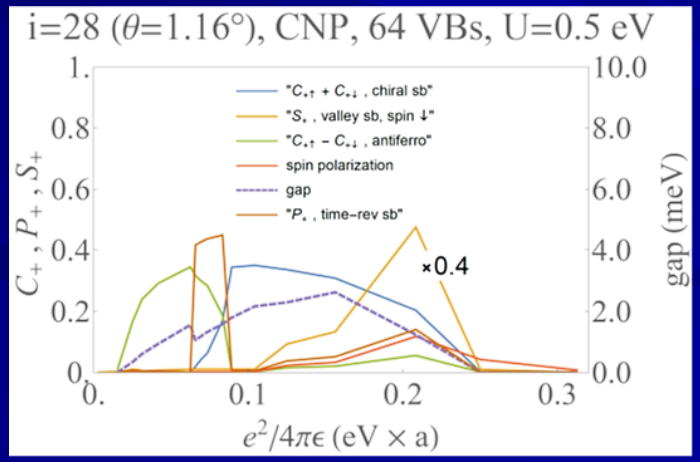
TIME-REVERSAL SYMMETRY BREAKING VS SPIN-POLARIZED PHASE

Therefore, **at the charge neutrality point,**

the value of the on-site repulsion U is a relevant scale which dictates whether there is **antiferromagnetic** order or not at weak coupling of the extended Coulomb interaction



$U = 4.0$ eV



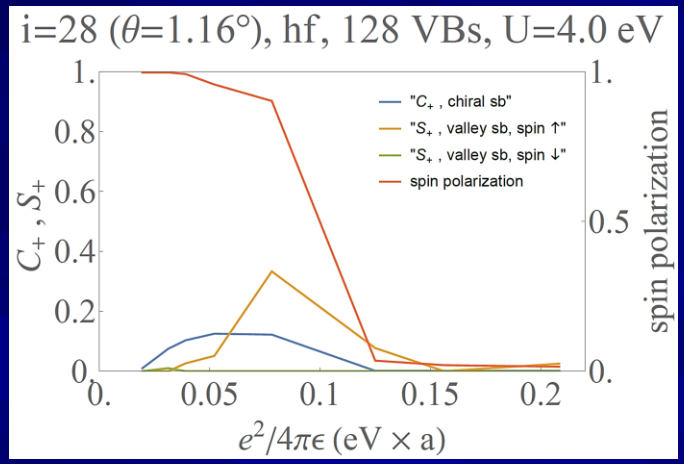
$U = 0.5$ eV

J. G. and T. Stauber,
arXiv:2103.09015

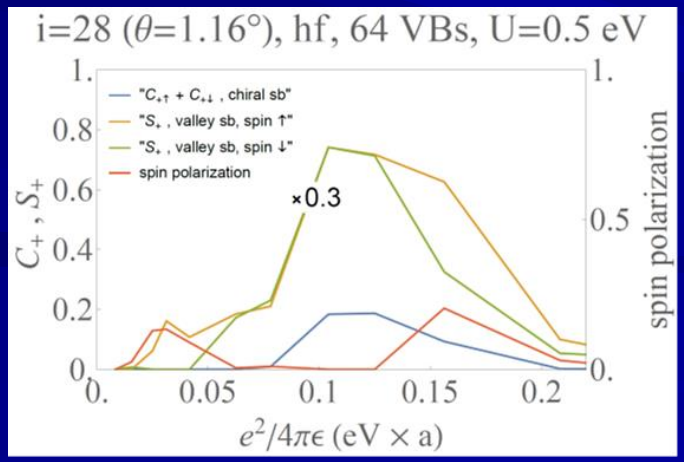
TIME-REVERSAL SYMMETRY BREAKING VS SPIN-POLARIZED PHASE

A**t half-filling** of the lowest valence band,

the value of the on-site repulsion U is a relevant scale which dictates whether there is **ferromagnetic** order or not at weak coupling of the extended Coulomb interaction



$U = 4.0$ eV

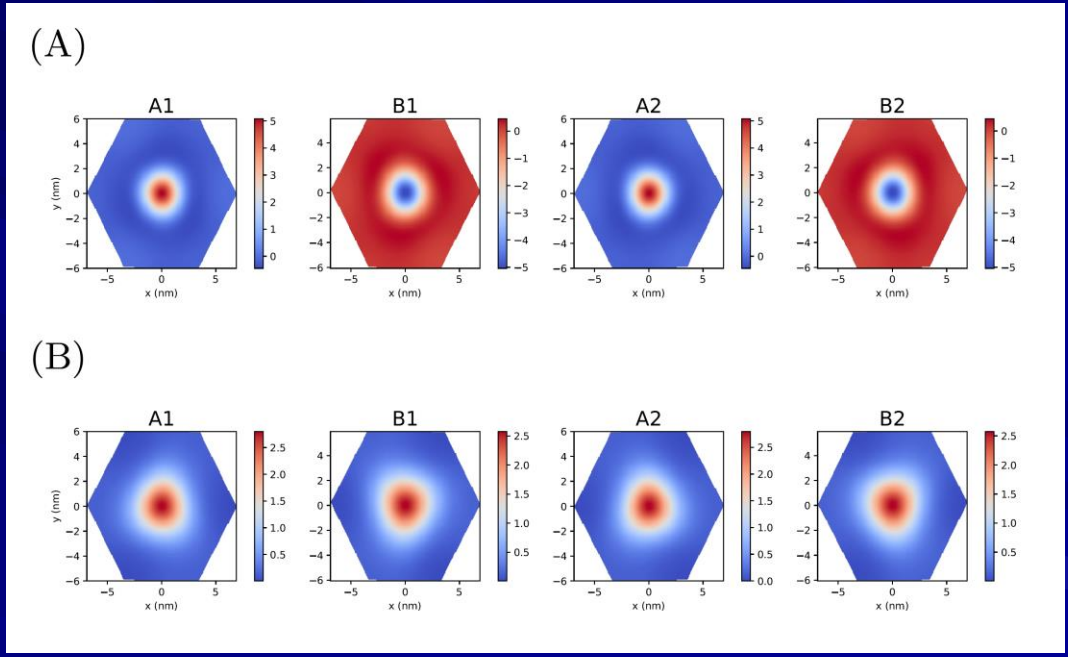


$U = 0.5$ eV

J. G. and T. Stauber,
arXiv:2103.09015

TIME-REVERSAL SYMMETRY BREAKING VS SPIN-POLARIZED PHASE

Those magnetic phases should lead to clear experimental signatures, since the spin density would be concentrated on the regions with stacking AA, in the antiferromagnetic state at the charge neutrality point (A) as well as in the ferromagnetic state at half-filling of the lowest valence band (B)



J. G. and T. Stauber,
arXiv:2103.09015

TIME-REVERSAL SYMMETRY BREAKING VS SPIN-POLARIZED PHASE

In conclusion, for sufficiently strong on-site (Hubbard) repulsion U and depending on the dielectric screening,

- an antiferromagnetic state may appear at the charge neutrality point
- a ferromagnetic state may arise at half-filling of the lowest valence or conduction band

These states should lead to clear experimental signatures, since the spin density would be concentrated on the regions with stacking AA, giving rise to a kind of “magnetic lattice”.