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Magnetic gap opening in rhombohedral stacked multilayer graphene from first principles[1] MATTEO CALANDRA, BETUL PAMUK, JACOPO BAIMA, CNRS, FRANCESCO MAURI, Universita di Roma La Sapienza — We investigate the occurrence of magnetic and charge density wave instabilities in rhombohedral stacked multilayer graphene by using hybrid functionals. Neglecting spin-polarization, an extremely flat surface band centered at the special point **K** of the Brillouin zone occurs at the Fermi level. Spin polarization opens a gap in the surface state by stabilizing an antiferromagnetic state. The top and the bottom surface layers are weakly ferrimagnetic in-plane and are antiferromagnetic coupled to each other. This coupling is propagated by the out-of-plane antiferromagnetic coupling between the nearest neighbors. The gap is very small in spin polarized generalized gradient approximation, it increases with larger amount of exact exchange. For trilayer rhombohedral graphene it is 38.6 meV in PBE0, in agreement with the 42 meV gap found in experiments. We study the temperature and doping dependence of the magnetic gap. Charge density wave instabilities with $\sqrt{3} \times \sqrt{3}$ periodicity do not occur.

References: Betul Pamuk, Jacopo Baima, Francesco Mauri, Matteo Calandra arXiv:1610.03445

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