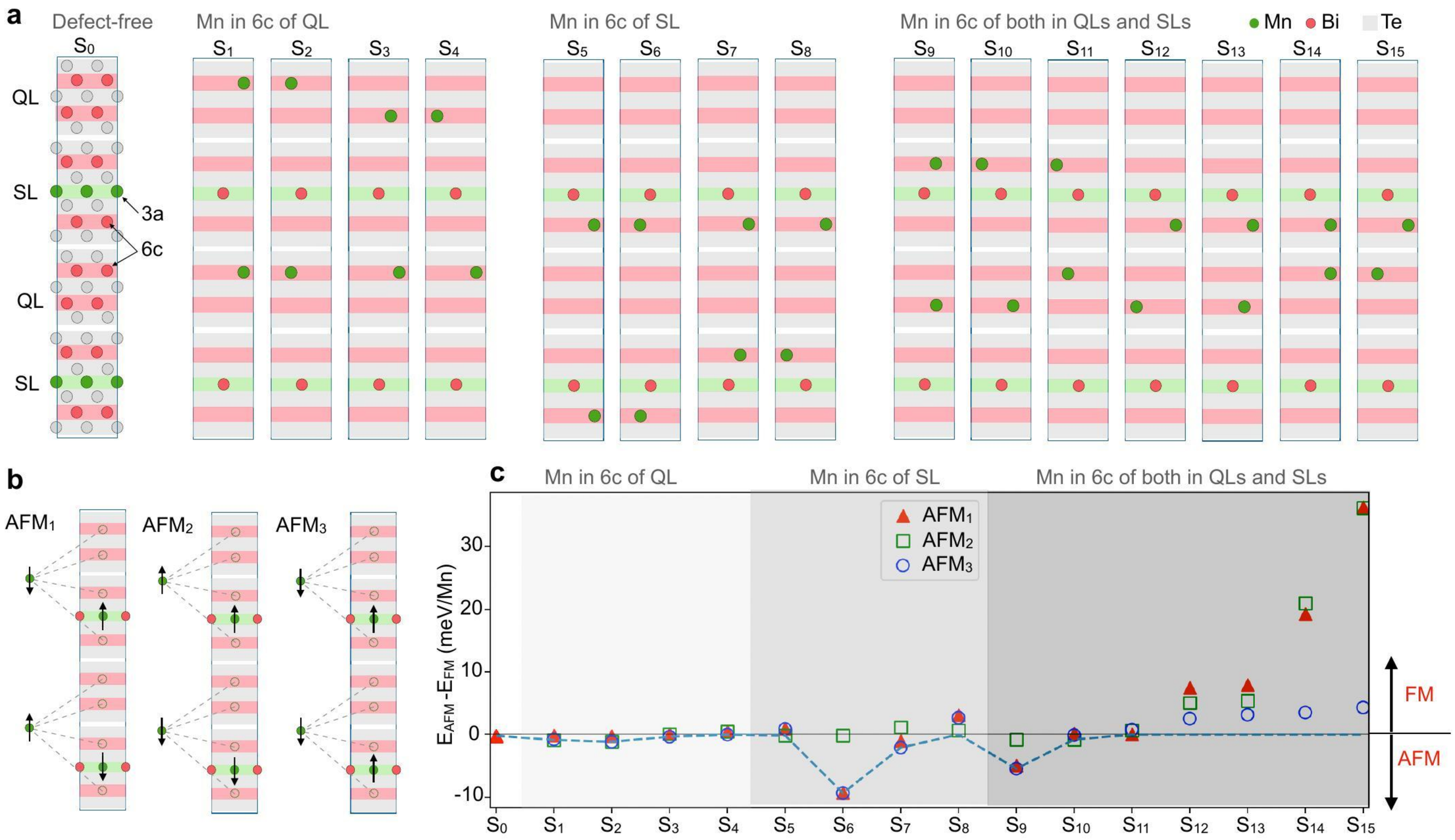

FIG. 3. Crystal- and magnetic-structure models and their DFT energies. (a) Schematics of the structure models with various Mn/Bi intermixing scenarios. S_0 is the defect-free case while the panels from S_1 to S_{15} visualize the structural differences to S_0. Models S_1 to S_4: antisite Mn (green) is in the 6*c* site of the QLs; models S_5 to S_8: antisite Mn is in the 6*c* site of the SLs; models S_9 to S_{15}: antisite Mn is in the 6*c* positions of both QLs and SLs. (b) Schematics of the constructed magnetic arrangements. Each model has a distinct order between the Mn magnetic moments in the 3*a* and 6*c* positions which are conditioned by the respective structure model in (a). Ferromagnetic order with an out-of-plane orientation of the moments is assumed within each atomic layer. (c) Total energy difference between an antiferromagnetic ordering model (1, 2 or 3) of each structure model (S_0 to S_{15}) and the respective fully ferromagnetic configuration, as obtained from the scalar-relativistic DFT calculations. The dashed line follows the ground state energy, zero corresponding to the FM phase.

gory antisite Mn occupy the 6*c* positions of *only* the SLs (S_5 to S_8). In the third category, the Mn atoms are distributed over the 6*c* positions of *both* the QLs and the SLs (S_9 to S_{15}).

For each structure model, we consider four possible magnetic arrangements: a fully spin-polarized FM order and three different AFM models sketched in Fig. 3b. They all have in common that the Mn moments order FM within any given atomic layer, but vary in the magnetic couplings between the adjacent atomic layers along the stack. In the AFM_1 and AFM_2 models, the Mn spins in the two consequent 3*a* positions are oppositely coupled. The coupling between the 3*a* site and all intermixed Mn neighbours in the 6*c* site(s) is either AFM (AFM_1) or FM (AFM_2), respectively. The AFM_3 model realises parallel spin arrangement in the 3*a* sites, while they couple AFM with the Mn defects in all 6*c* positions.

Fig. 3c discerns what is an energetically favorable magnetic arrangement for each considered structure model of $MnBi_4Te_7$ as compared to the fully spin-polarized FM state. For a given model, if any AFM model obeys $E_{AFM} - E_{FM} < 0$, we conclude that antiferromagnetism is preferred. On the other hand, if all AFM models fulfill $E_{AFM} - E_{FM} > 0$, we define the fully FM phase as the ground state.

A clear trend in the magnetic order as a function of the underlying Mn/Bi intermixing pattern can be established. All but one models of the first two categories, where the intermixed Mn cations occupy *either* the SLs *or* the QLs, show an AFM configuration as the lower energy state. This preference reverts markedly if the antisite Mn distributes over the 6*c* positions of *both* the QLs and the SLs: five out of the seven constructed structure configurations of this category prefer the FM phase. A closer look reveals that the preference for the FM state is particularly prominent in those structure models (S_{12} to S_{15}), in which the Mn cations occupy the nearby 6*c* positions not separated by the 3*a* positions – namely, when continuous magnetic exchange pathways exist between the antisite Mn ions.

These results establish a strong correlation between the magnetic structure and the Mn distribution along the stacking direction. When an antisite Mn is located only in one of the two 6*c* positions of the QLs – a situation ex-