Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Engineering antiferromagnetic topological insulator in two-dimensional NaMnBi

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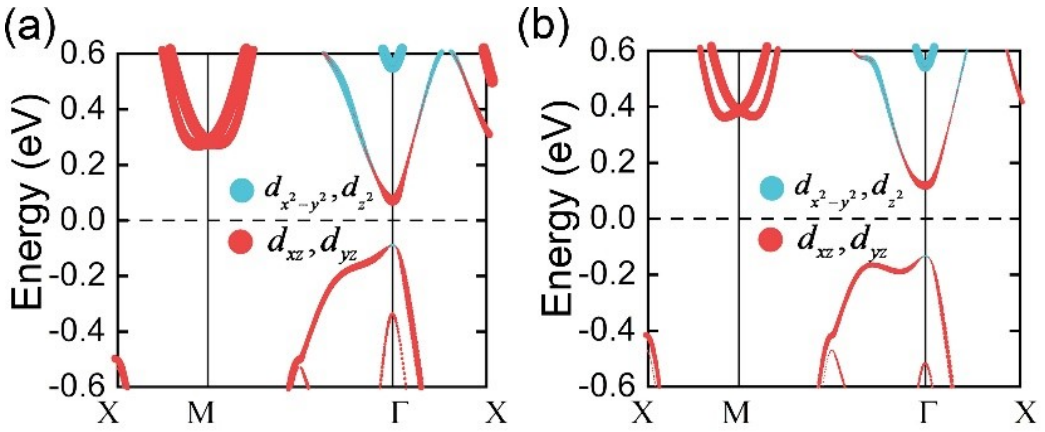

Figure S1. Band structures of NaMnBi QL under a 2% compressive strain with (a) U = 3 eV and (b) U = 5 eV. The bands are weighted with the contribution of $Mn-d_{z^2}$ / $d_{x^2-y^2}$ and $Mn-d_{xz/yz}$ orbitals, indicating the band inversion at the Γ point for all of the considered U values. The fermi level is indicated with a dashed line.

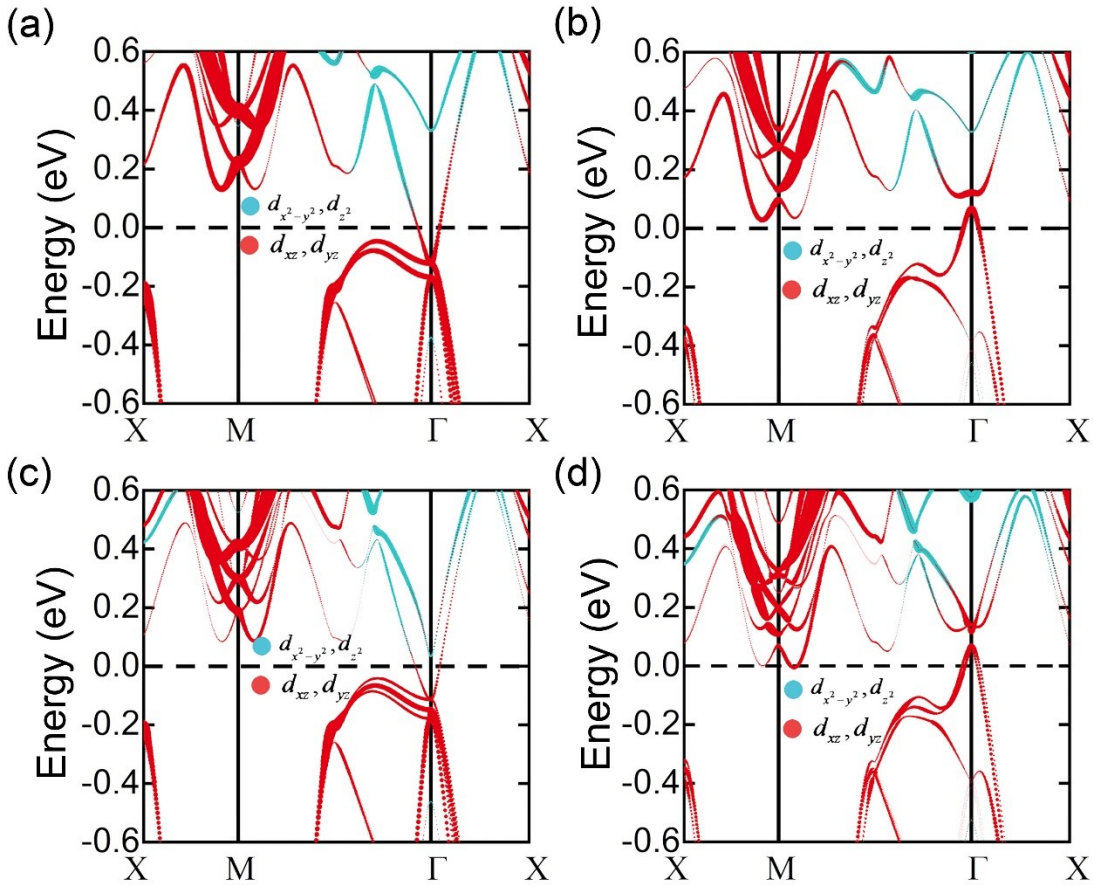

Figure S2. Orbitally resolved band structures of (a), (b) bilayer system and (c), (d) trilayer system (a), (c) without and (b), (d) with SOC, weighted with the contribution of $Mn-d_{z^2}/d_{x^2-y^2}$ and $Mn-d_{xz/yz}$ orbitals. The fermi level is indicated with a dashed line.

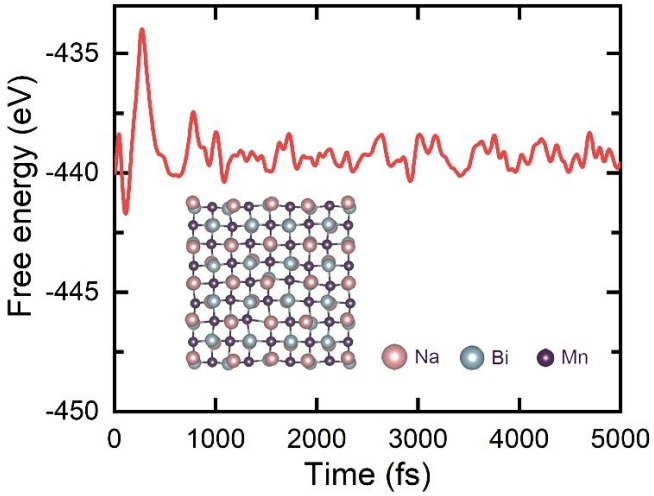

Figure S3. Variation of the free energy with 0-5000 fs for NaMnBi. Ab Initio Molecular Dynamics (AIMD) simulation is carried with a 4*4*1 supercell under 300 K. The inset is the snapshot taken from the end of AIMD calculation and neither broken bonds nor structure reconstruction occur during the whole time interval.