Supporting Information

TMB (TM=Cr, Fe) Monolayers: A new Type of Room Temperature Antiferromagnetic Topological Nodal Line Semimetals

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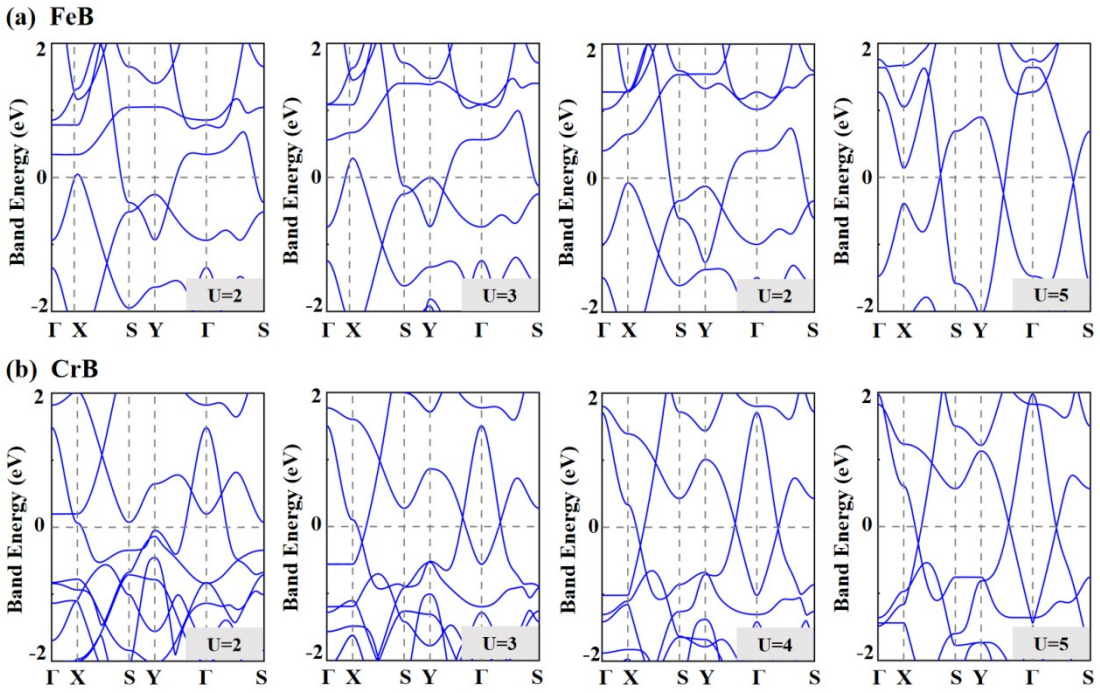

Fig. S1. (a) Band structures of FeB monolayer with different U values added. (b) Band structures of CrB monolayer with different U values added.

TABLE S1. The elastic constants of C_{11}, C_{12}, C_{22}, and C_{66} for FeB and CrB monolayers.

System	C_{11} (N/m)	C_{12} (N/m)	C_{22} (N/m)	C_{66} (N/m)
FeB	740.6917	413.7599	740.374	608.9664
CrB	524.5973	378.0358	524.6856	444.3339

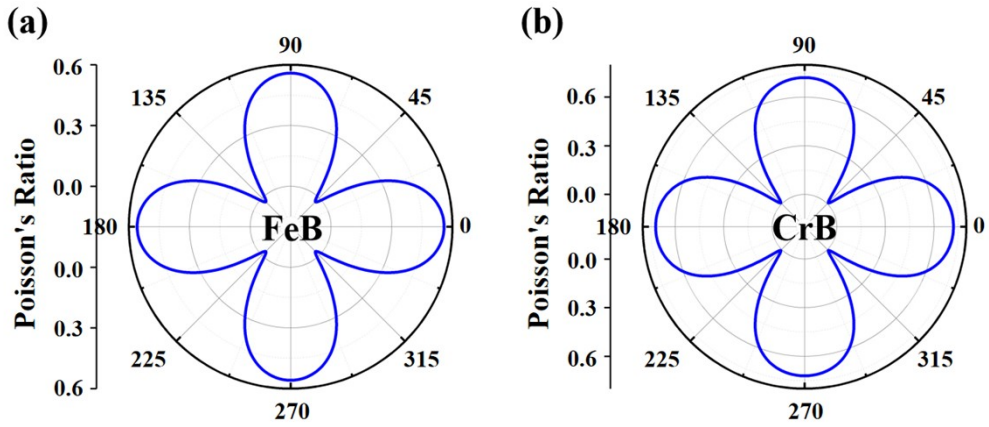

Fig. S2. Poisson's ratios of the FeB (a) and CrB (b) monolayers.

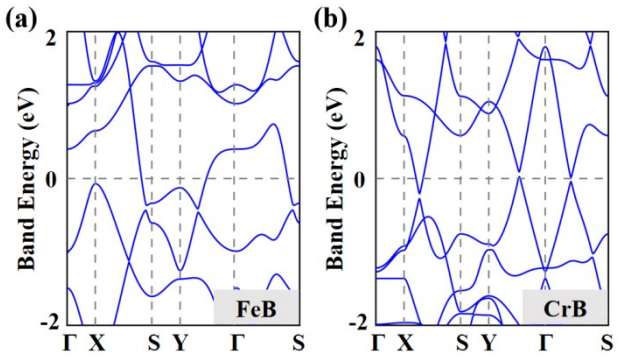

Fig. S3. The band structure of (a) FeB and (b) CrB monolayers with SOC applied along the z-direction.

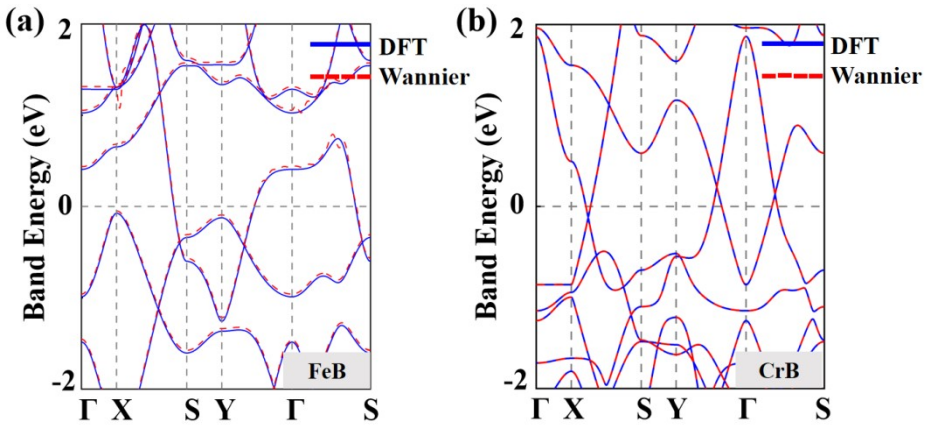

Fig. S4. Band structure of FeB (a) and CrB (b), and blue solid line and red dotted line are the results under DFT calculations and tight-binding model.

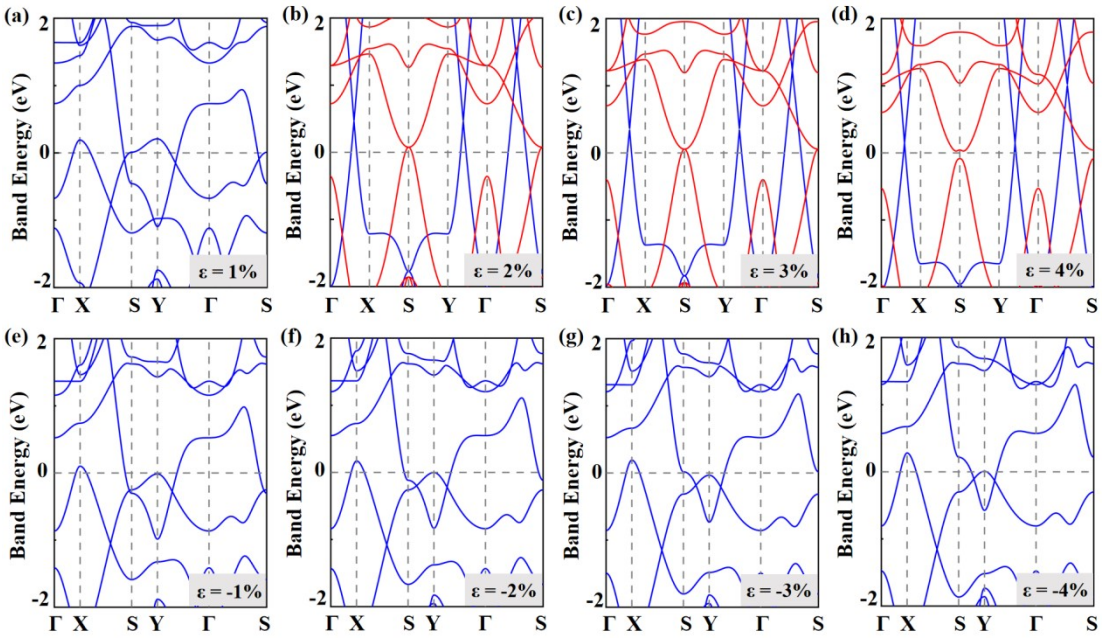

Fig. S5. The band structure of FeB monolayers in the range of ε = - 4% to 4%.

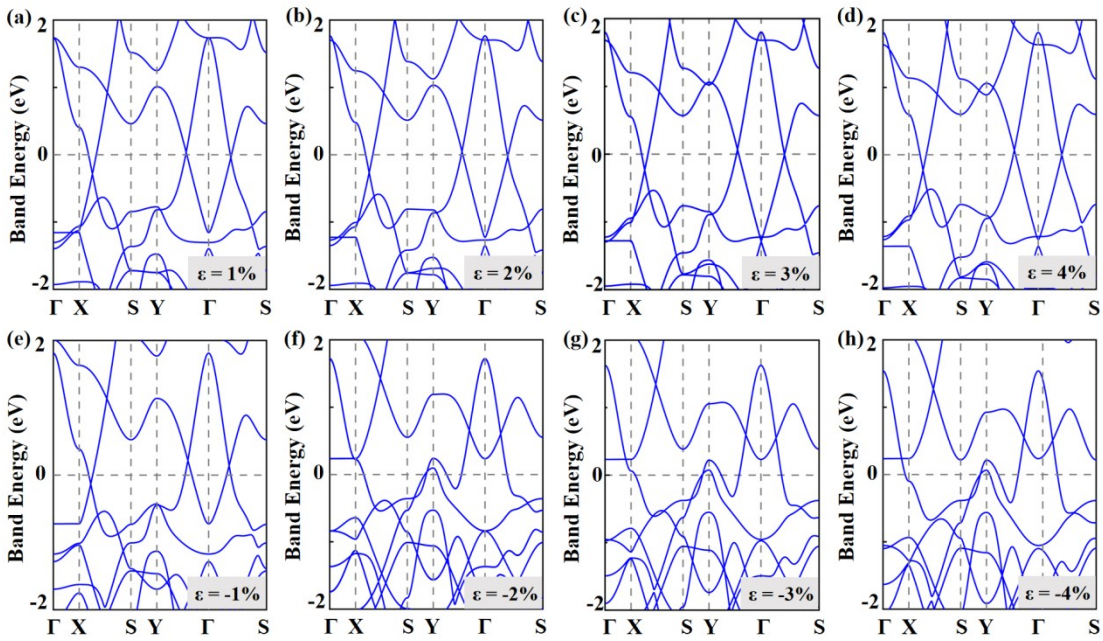

Fig. S6. The band structure of CrB monolayers in the range of ε = - 4% to 4%.

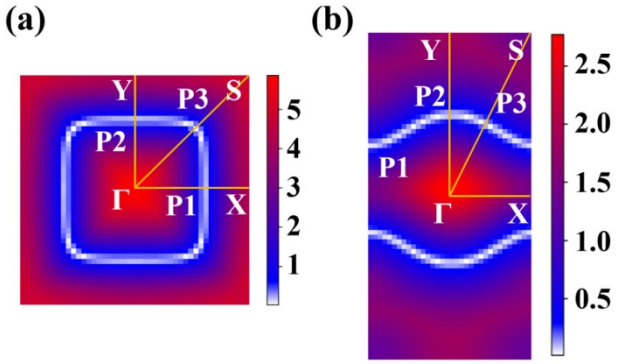

Fig. S7. The diagram of the gap size at Fermi level in BZ of FeB monolayer under tensile 2% strain (a) and CrB monolayer under tensile 3% strain (b).