

Supporting information for

Decomposition and Phase Transformation of Ti_2AlN MAX Thin Film Upon Annealing in Ultra-high-vacuum

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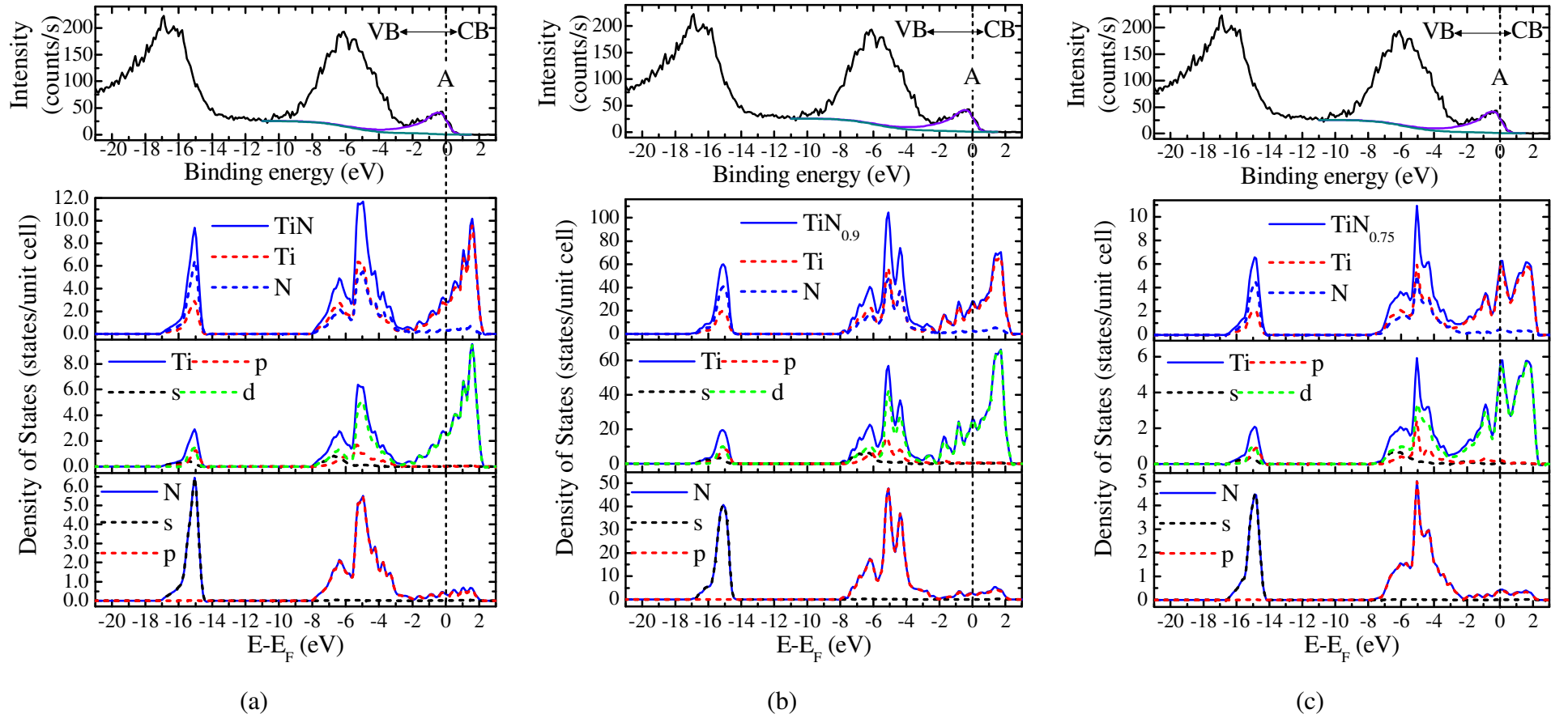


Figure S1. Partial density of states (PDOS) and total density of states (TDOS) calculated by density function theory (DFT) from (a) a perfect $1 \times 1 \times 1$ TiN structure, (b) TiN_{0.9} represented by removing three N atoms from $2 \times 2 \times 2$ TiN and (c) TiN_{0.75} represented by removing one N atom from $1 \times 1 \times 1$ TiN supercell structure.