

Supplementary Material

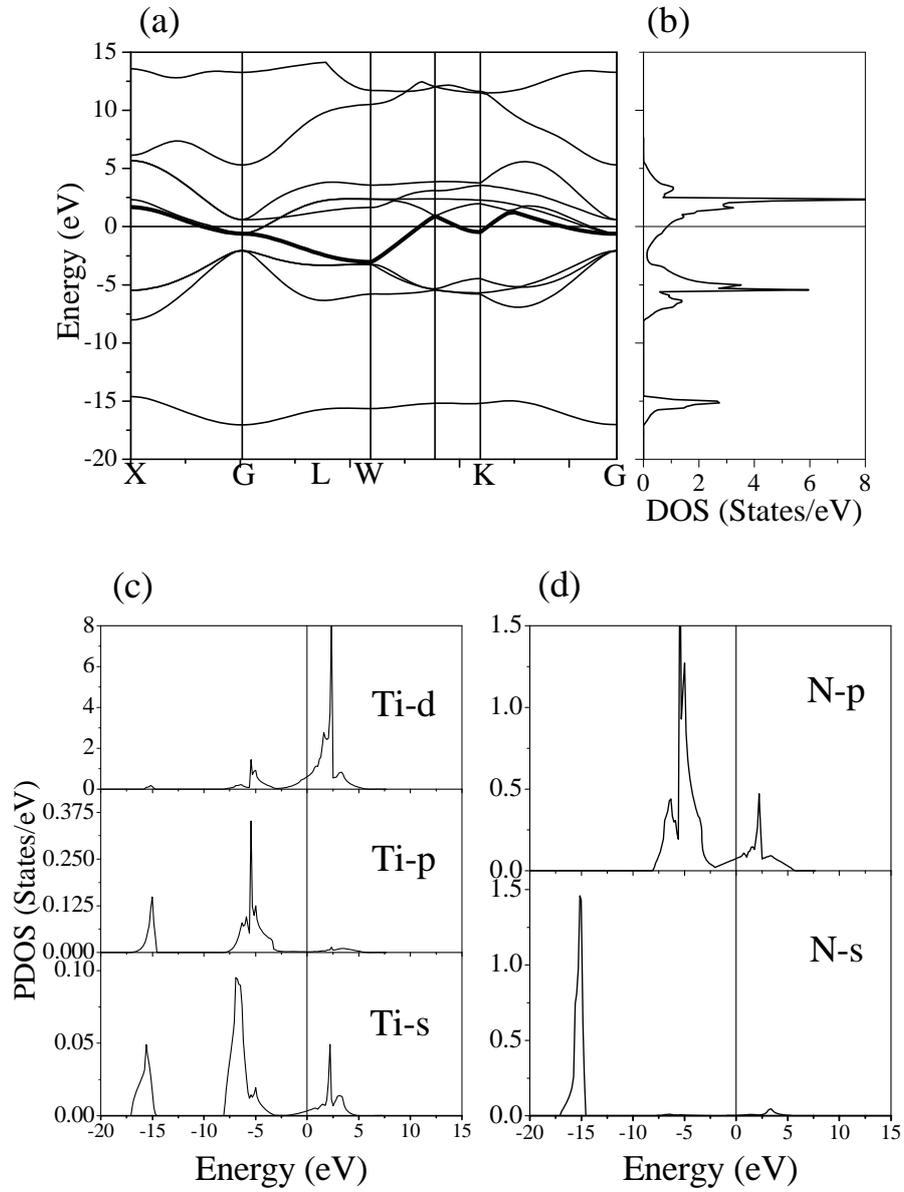


Figure S1. Band structure, density of state (DOS) and partial density of state (PDOS) of B1-NaCl structure of TiN. (a) Band structure, (b) density of state (DOS), (c) partial density of state of Ti atom, and (d) PDOS of N atom.

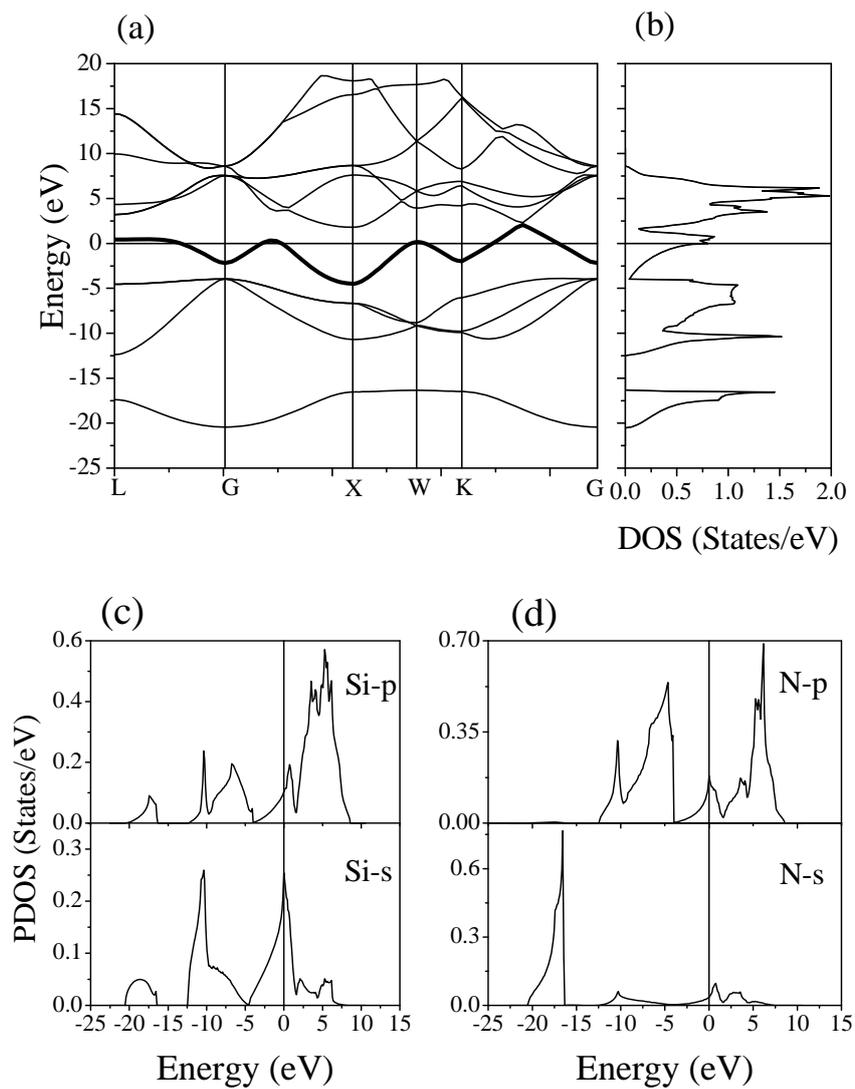


Figure S2. Band structure, density of state (DOS) and partial density of state (PDOS) of B1-NaCl structure of B1-SiN. (a) Band structure, (b) density of state (DOS), (c) partial density of state of Si atom, and (d) PDOS of N atom.

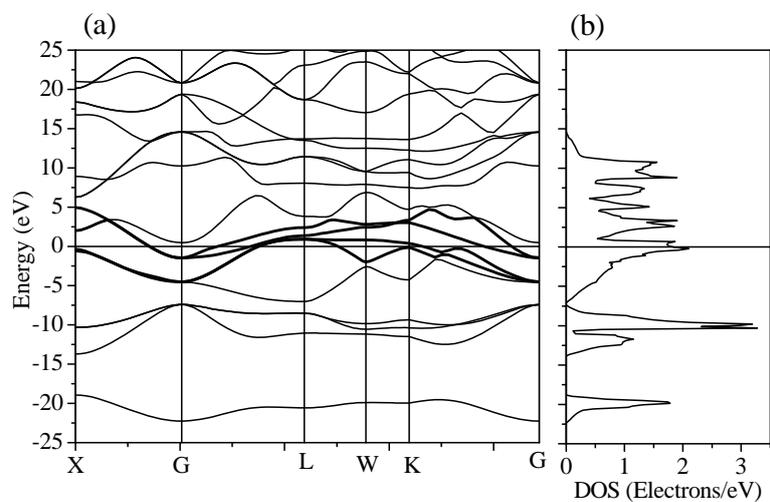


Figure S3. Cont.

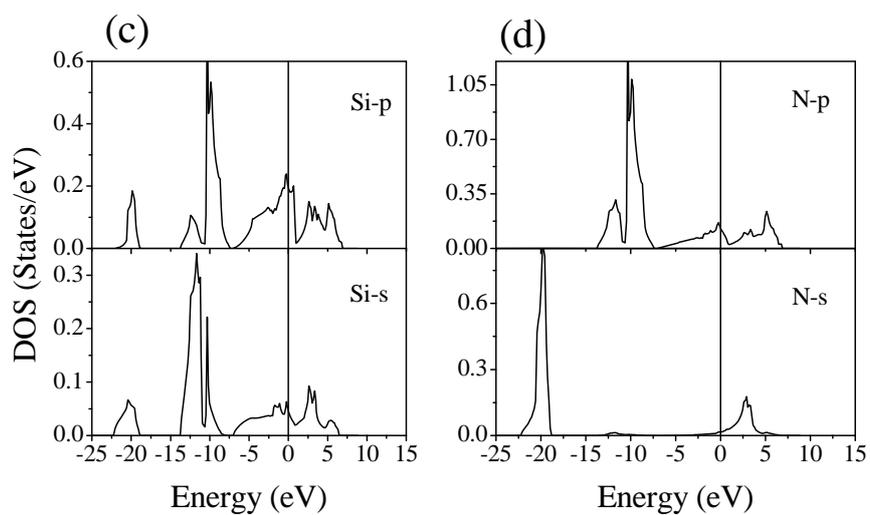


Figure S3. Band structure, density of state (DOS) and partial density of state (PDOS) of 1Si-4N4Ti. (a) Band structure, (b) density of state (DOS), (c) partial density of state of Si atom, and (d) PDOS of N atom.