Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Modifying the Electronic and Magnetic Properties of Scandium Nitride Semiconductor Monolayer via Vacancy and Doping

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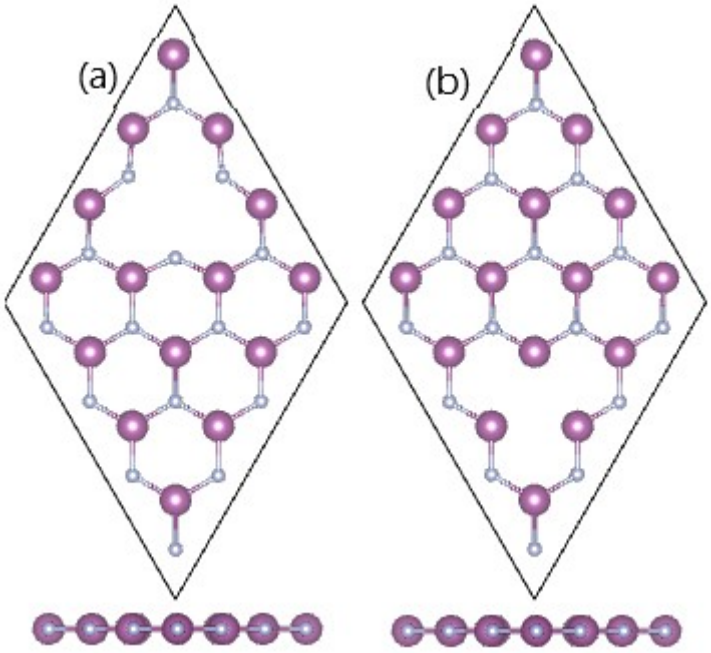

Figure S1: Relaxed atomic structure of ScN monolayer with (a) Single Sc vacancy and (b) Single N vacancy.

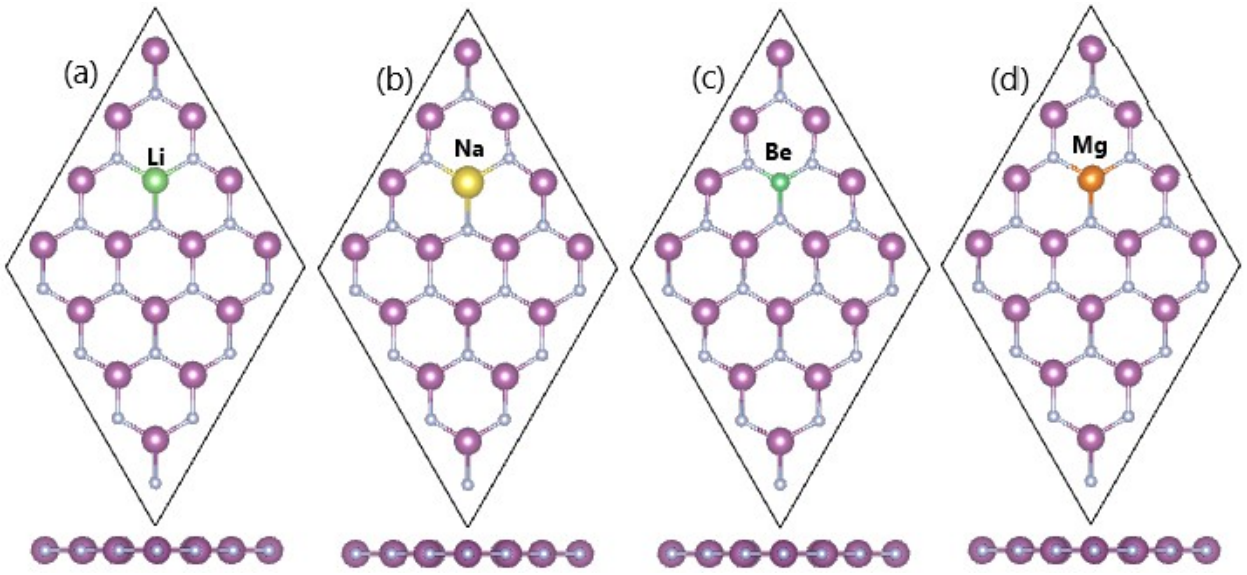

Figure S2: Relaxed atomic structure of (a) Li-, (b) Na-, (c) Be-, and (d) Mg-doped ScN monolayer.

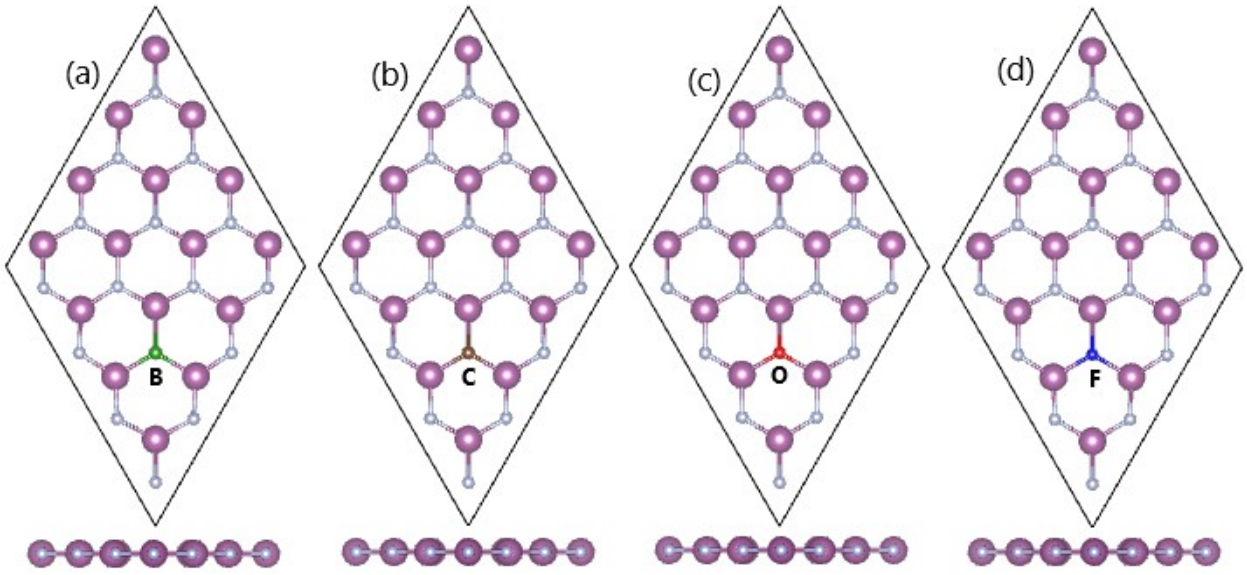

Figure S3: Relaxed atomic structure of (a) B-, (b) C-, (c) O-, and (d) F-doped ScN monolayer.

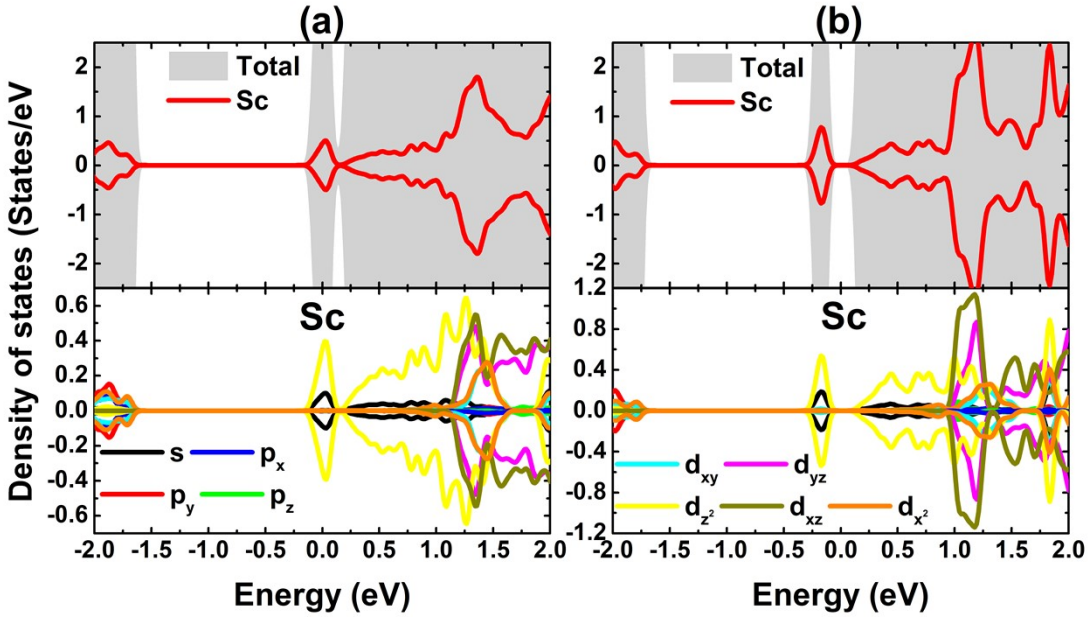

Figure S4: Total and projected density states of Sc atom closest to doping site of (a) O- and (b) F-doped ScN monolayer.

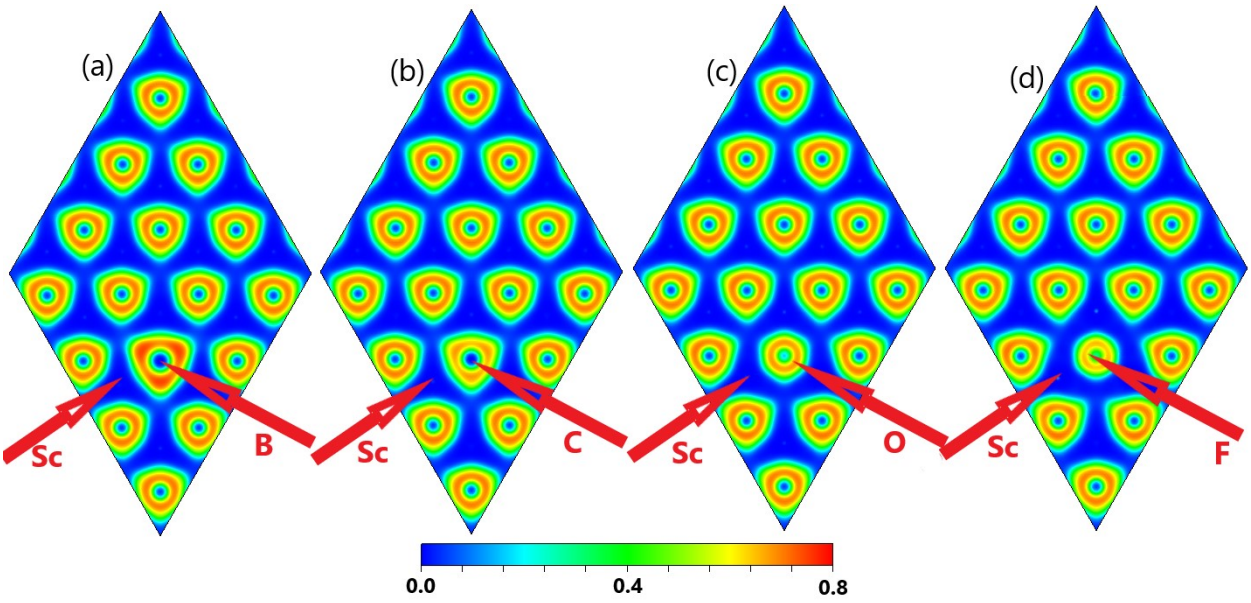

Figure S5: Electron localization function in (a) B-, (b) C-, (c) O-, and (d) F-doped ScN monolayer.

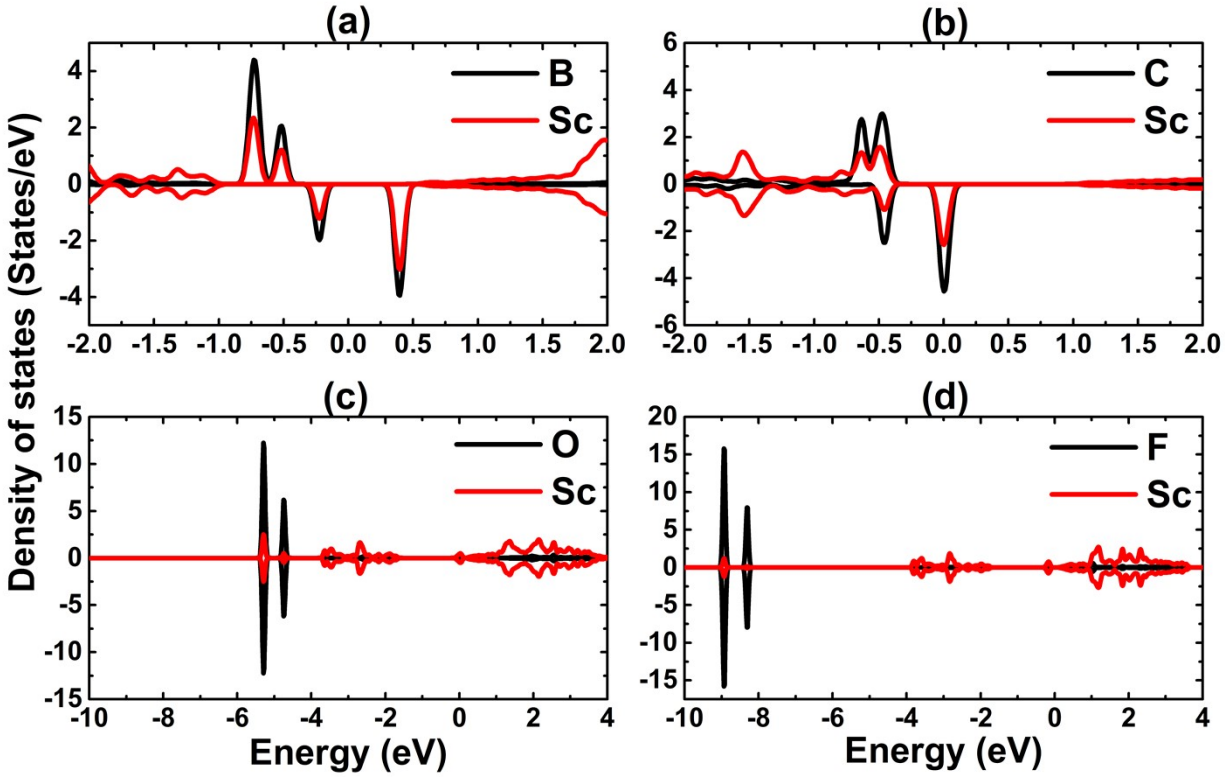

Figure S6: Atom-decomposed density of states of impurity and its neighbor Sc atom in (a) B-, (b) C-, (c) O-, and (d) F-doped ScN monolayer.