

Supplemental Material

Superconducting properties in doped 2M-WS₂ from first principles

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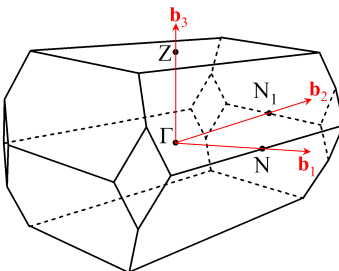


FIG. S1. Brillouin zone of 2M-WS₂ with high symmetry points.

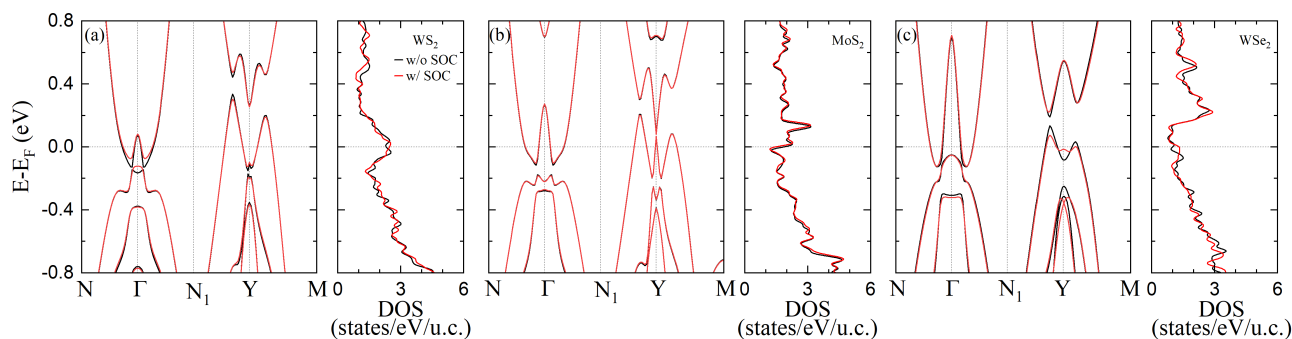


FIG. S2. Calculated electronic band structure and DOS of (a) WS₂, (b) MoS₂, and (c) WSe₂ for the 2M phase with and without using spin orbit coupling (SOC). An opening of the bands can be observed in the WS₂ due to the effect of SOC at Γ around 0.1 eV below the Fermi level.

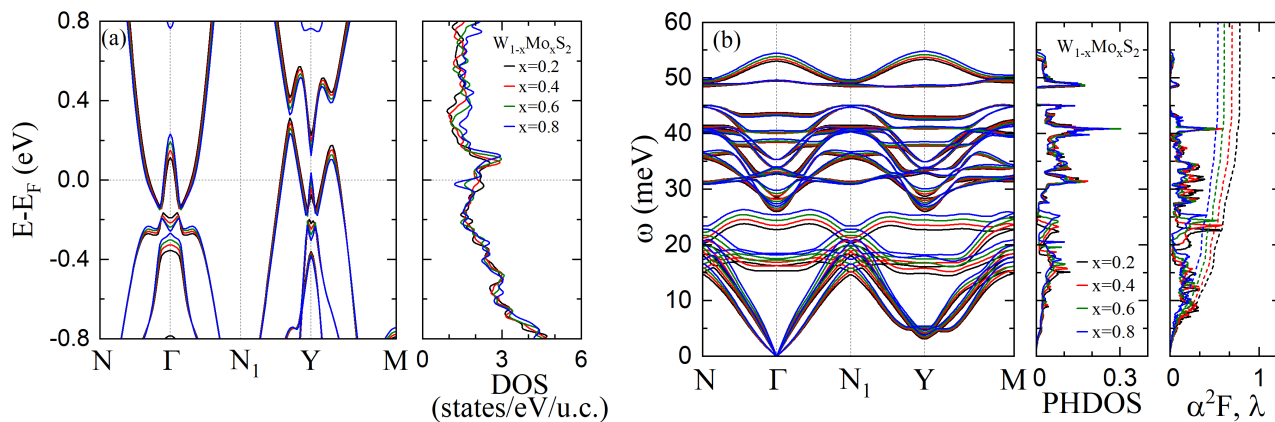


FIG. S3. (a) Calculated electronic band structure and DOS and (b) phonon dispersion, PHDOS, Eliashberg spectral function $\alpha^2F(\omega)$, and electron-phonon coupling strength λ of 2M-W_{1-x}Mo_xS₂ for various doping levels.

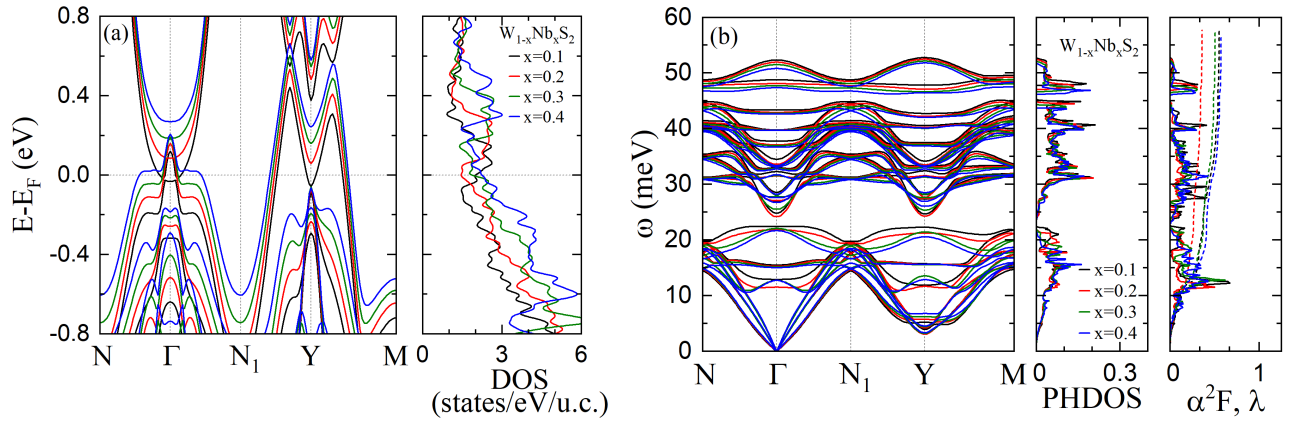


FIG. S4. (a) Calculated electronic band structure and DOS and (b) phonon dispersion, PHDOS, Eliashberg spectral function $\alpha^2F(\omega)$, and electron-phonon coupling strength λ of $2M-W_{1-x}Nb_xS_2$ for various doping levels.

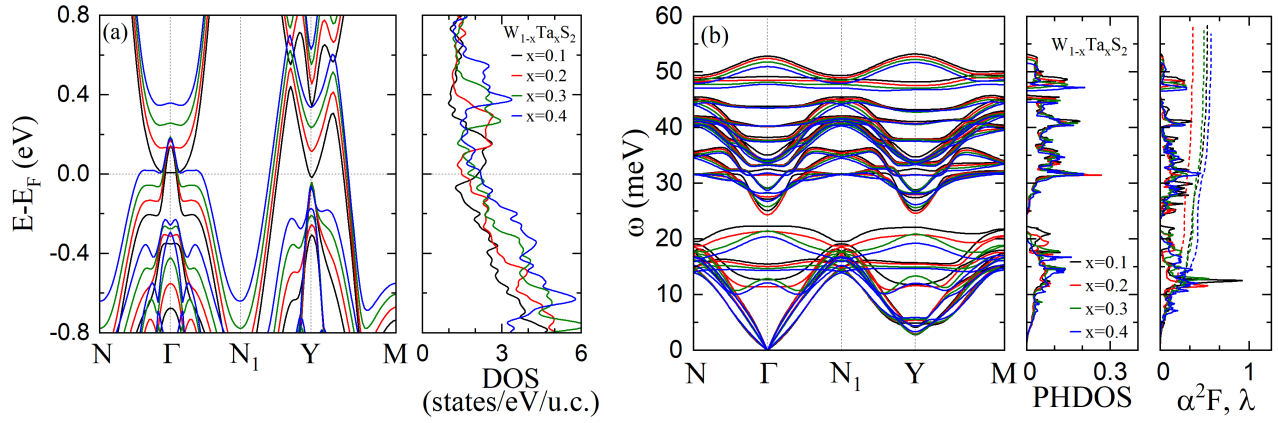


FIG. S5. (a) Calculated electronic band structure and DOS (states/eV/u.c.), (b) phonon dispersion, PHDOS, Eliashberg spectral function $\alpha^2F(\omega)$, and electron-phonon coupling strength λ of $2M-W_{1-x}Ta_xS_2$ for various doping levels.

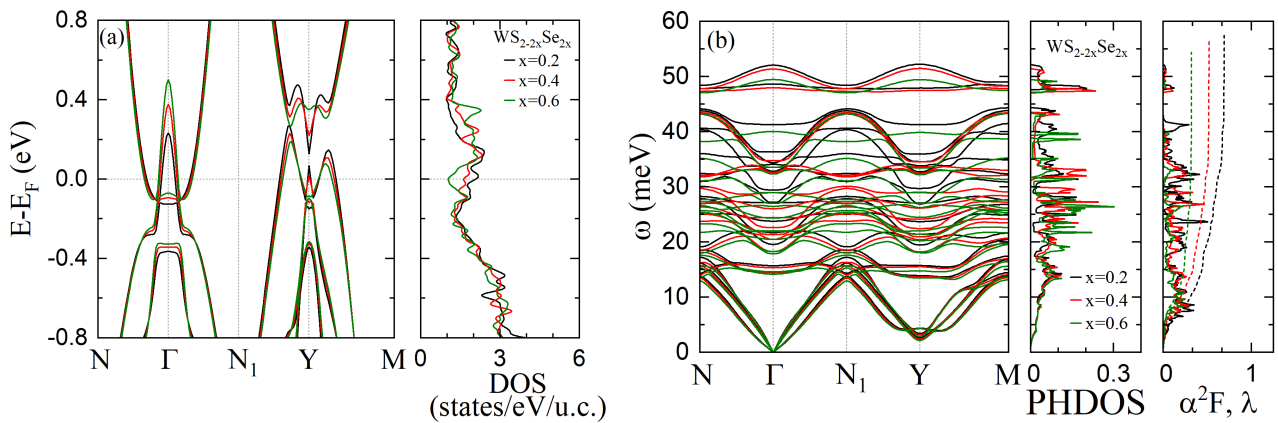


FIG. S6. (a) Calculated electronic band structure and DOS and (b) phonon dispersion, PHDOS, Eliashberg spectral function $\alpha^2F(\omega)$, and electron-phonon coupling strength λ of $2M-WS_{2(1-x)}Se_{2x}$ for various doping levels.

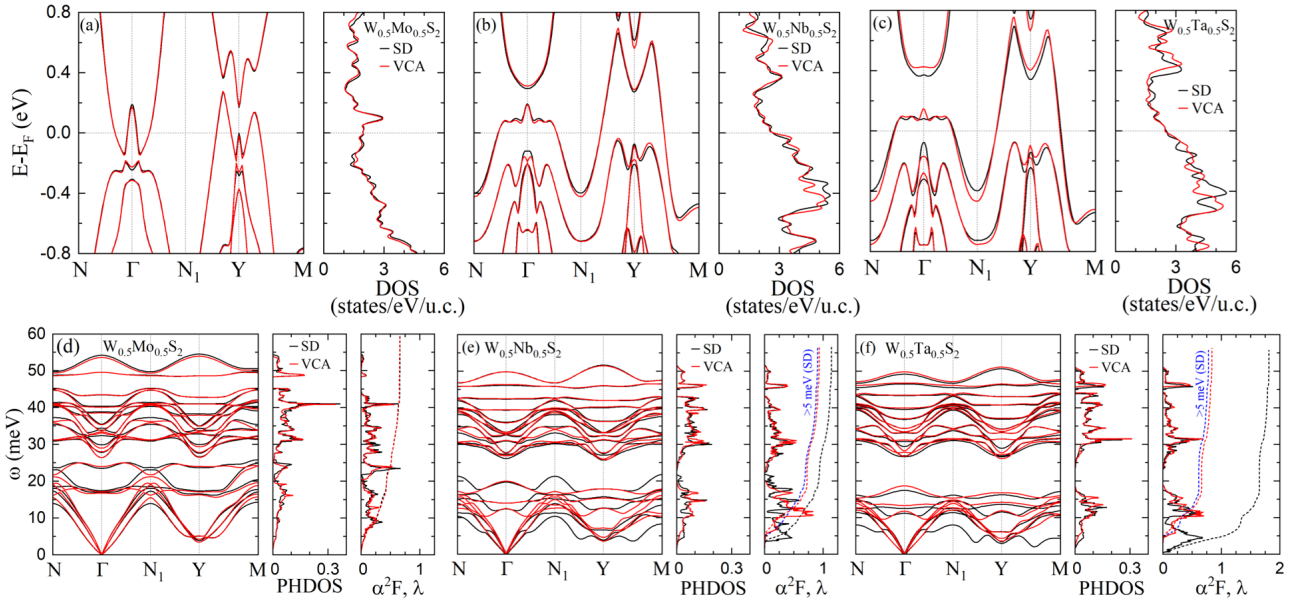


FIG. S7. (a-c) Electronic band structure and DOS and (d-f) phonon dispersion, PHDOS, Eliashberg spectral function $\alpha^2F(\omega)$, and electron-phonon coupling strength λ of 2M- $W_{0.5}M_{0.5}S_2$ (M = Mo, Nb, and Ta) calculated using the substitutional doping (SD) (black) and VCA (red) methods.

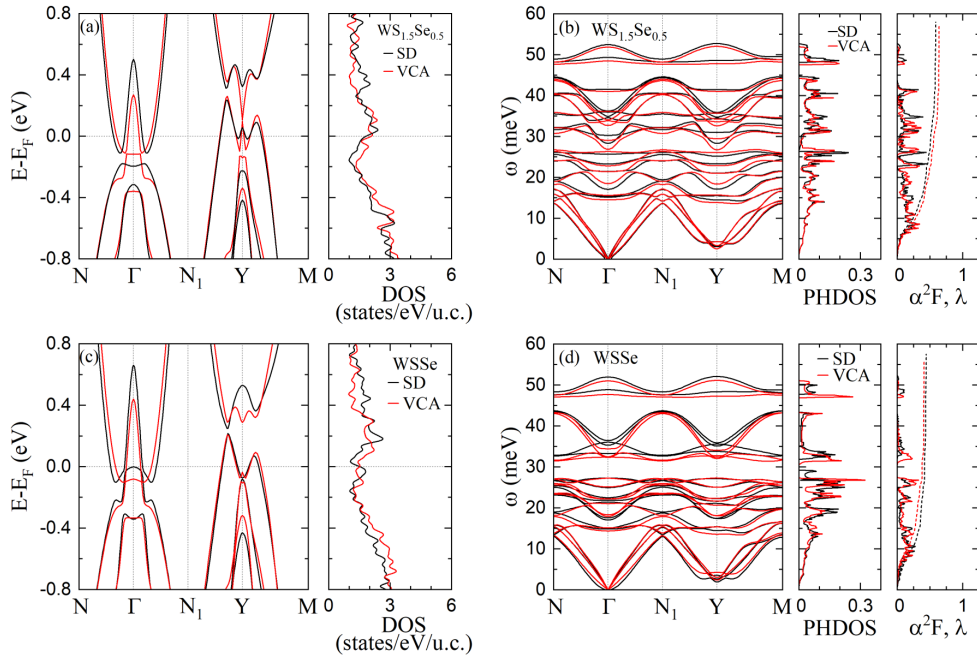


FIG. S8. (a, c) Electronic band structure and DOS and (b, d) phonon dispersion, PHDOS, Eliashberg spectral function $\alpha^2F(\omega)$, and electron-phonon coupling strength λ of 2M- $WS_{1.5}Se_{0.5}$ (top row) and 2M-WSSe (bottom row) calculated using the substitutional doping (SD) (black) and VCA (red) methods.