

Supporting information for: Electron-phonon coupling and hot electron thermalization in titanium nitride

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DFT results for gold and all the TiN systems considered: Au, TiN_{0.80}O_{0.20}, TiN_{0.85}O_{0.15}, TiN_{0.90}O_{0.10}, TiN_{0.95}O_{0.05}, TiN_{1.00}, TiN_{0.97}, TiN_{0.94}, TiN_{0.91}, TiN_{0.88}, TiN_{0.84}. TiN systems have been ordered with respect to the number of electrons per unit cell.

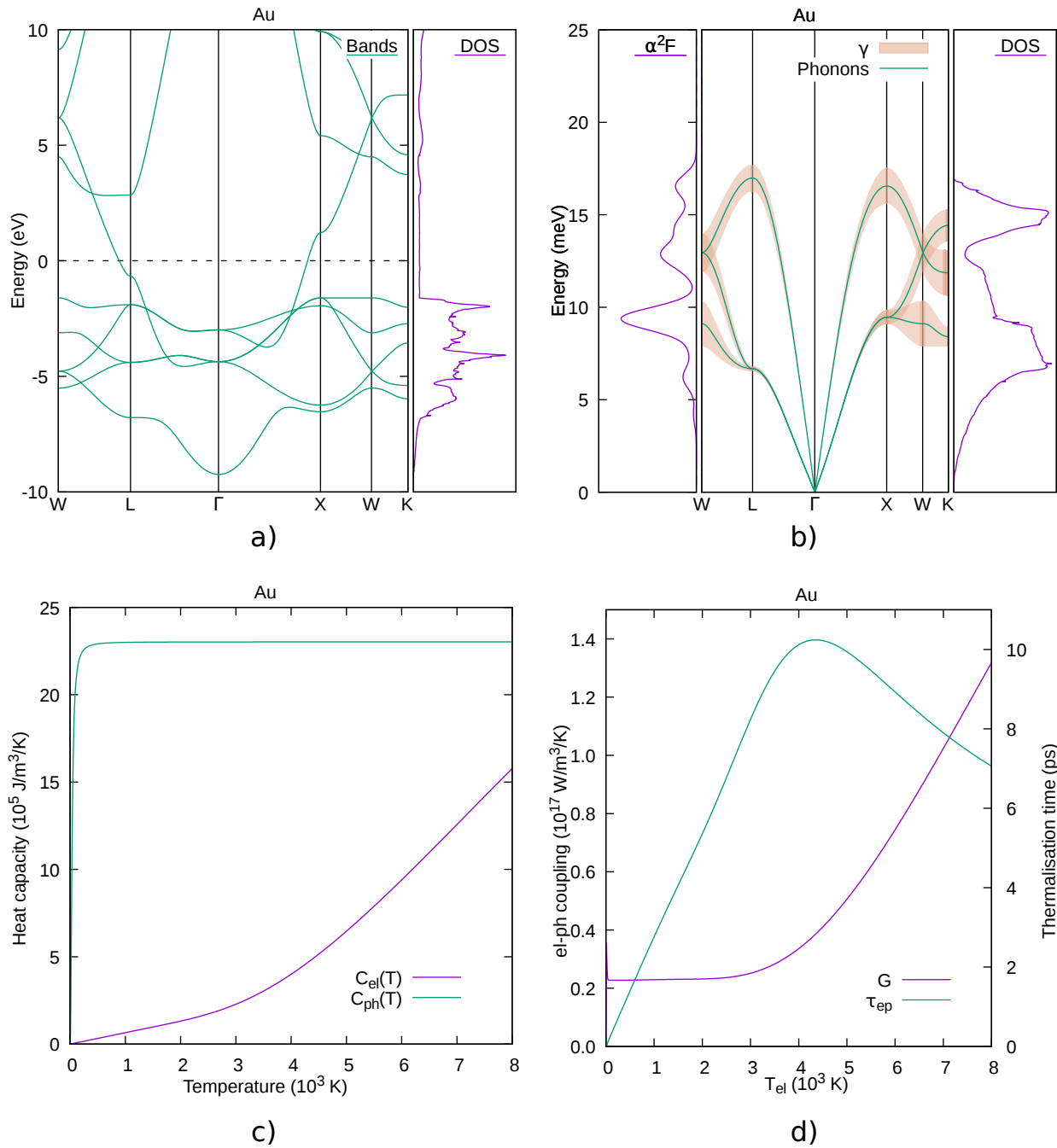


Figure S1: DFT results for Au. a) Electron band structure and DOS (DOS values in the range 0 to 5 states/eV/unitcell). b) Phonon band structure, DOS, phonon linewidths (magnification $\times 200$) and Eliashberg function (DOS and α^2F in the range 0 to 0.06 states/eV/unitcell and 0 to 0.3, respectively). c) Electron and phonon heat capacities. d) Electron-phonon coupling parameter and hot electron thermalisation time.

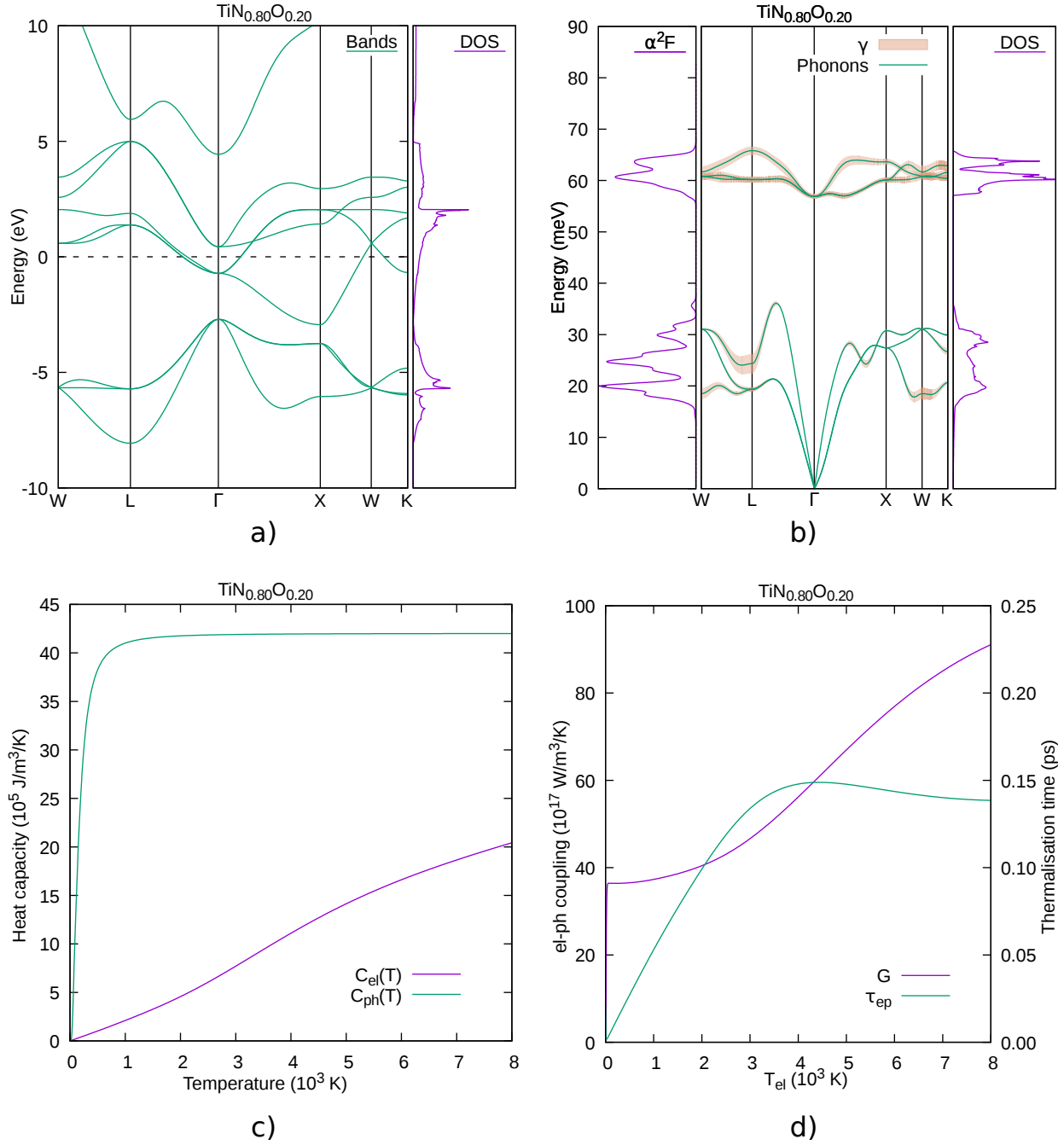


Figure S2: DFT results for $\text{TiN}_{0.80}\text{O}_{0.20}$. a) Electron band structure and DOS (DOS values in the range 0 to 16 states/eV/unitcell). b) Phonon band structure, DOS, phonon linewidths (magnification $\times 2$) and Eliashberg function (DOS and α^2F in the range 0 to 0.12 states/eV/unitcell and 0 to 1.3, respectively). c) Electron and phonon heat capacities. d) Electron-phonon coupling parameter and hot electron thermalisation time.

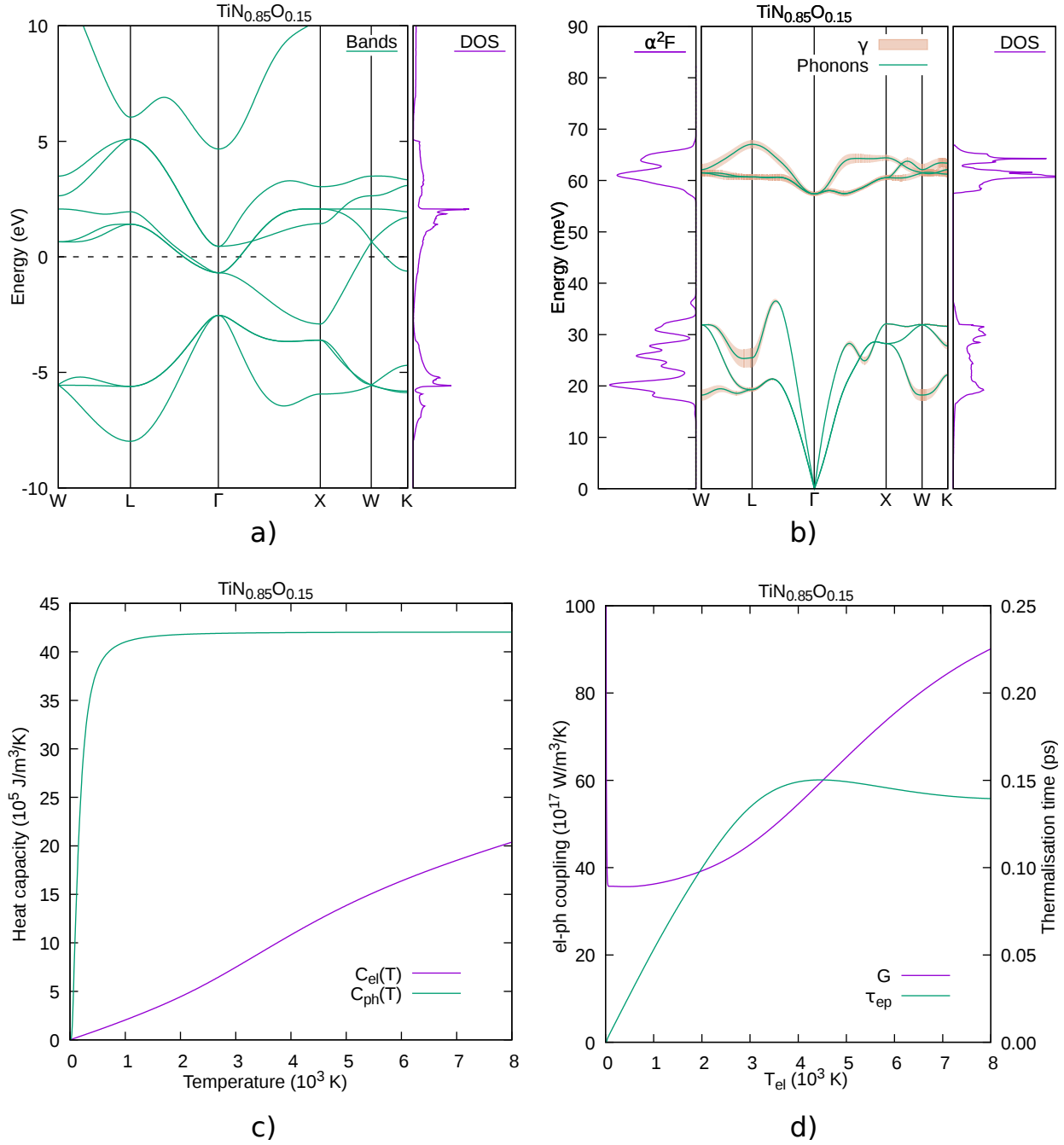


Figure S3: DFT results for $\text{TiN}_{0.85}\text{O}_{0.15}$. a) Electron band structure and DOS (DOS values in the range 0 to 16 states/eV/unitcell). b) Phonon band structure, DOS, phonon linewidths (magnification $\times 2$) and Eliashberg function (DOS and α^2F in the range 0 to 0.12 states/eV/unitcell and 0 to 1.3, respectively). c) Electron and phonon heat capacities. d) Electron-phonon coupling parameter and hot electron thermalisation time.

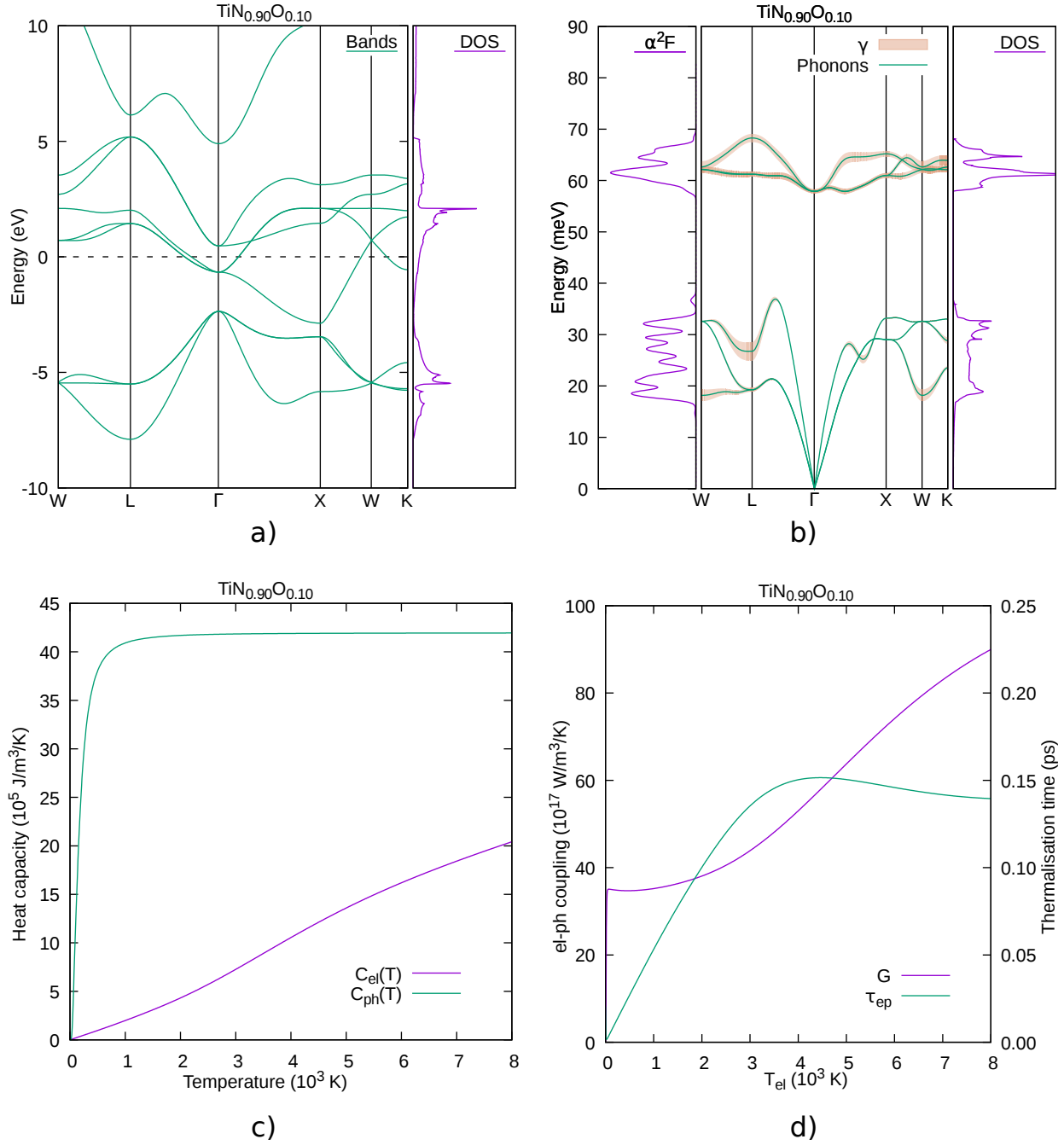


Figure S4: DFT results for $\text{TiN}_{0.90}\text{O}_{0.10}$. a) Electron band structure and DOS (DOS values in the range 0 to 16 states/eV/unitcell). b) Phonon band structure, DOS, phonon linewidths (magnification $\times 2$) and Eliashberg function (DOS and α^2F in the range 0 to 0.12 states/eV/unitcell and 0 to 1.3, respectively). c) Electron and phonon heat capacities. d) Electron-phonon coupling parameter and hot electron thermalisation time.

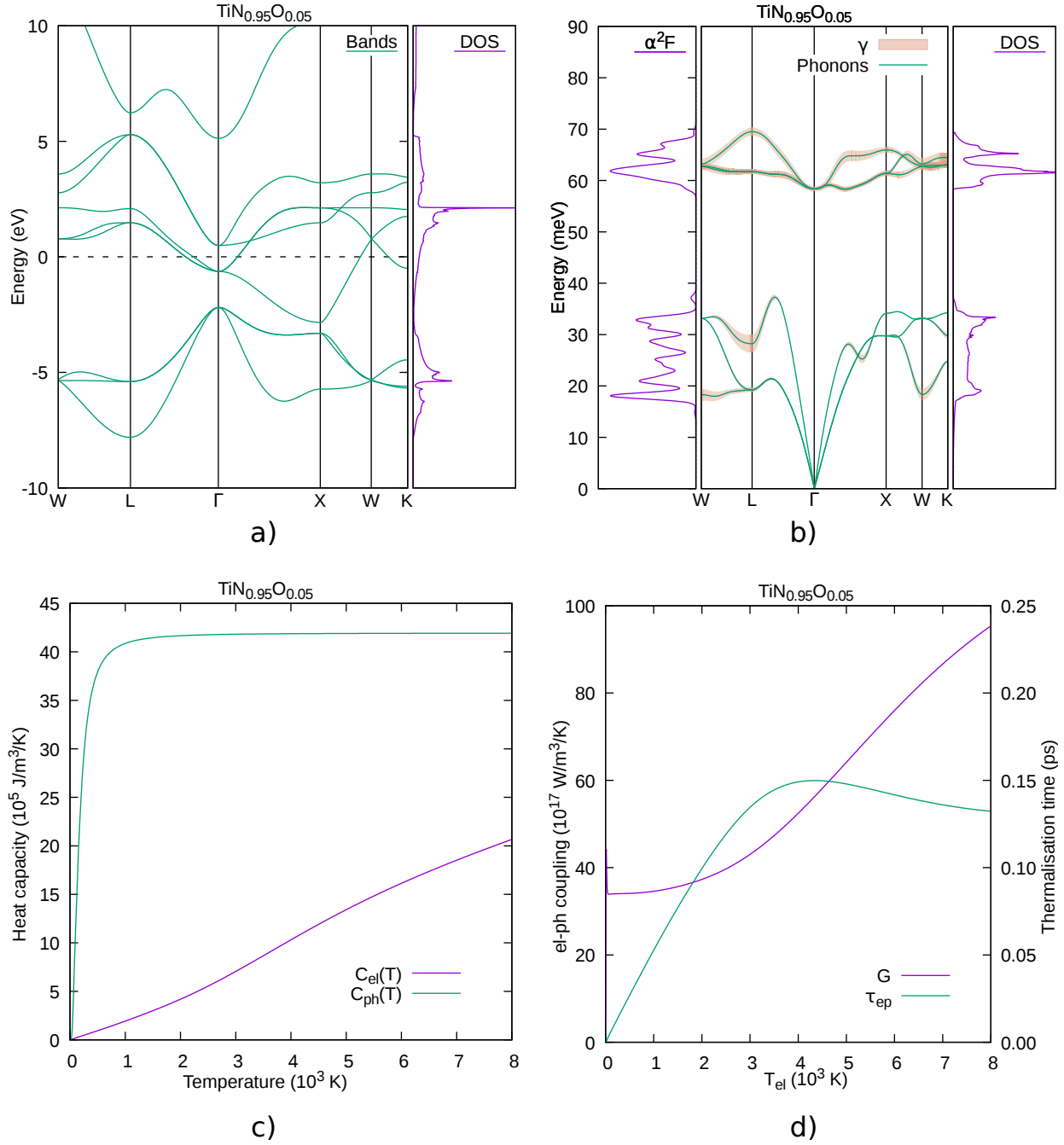


Figure S5: DFT results for $\text{TiN}_{0.95}\text{O}_{0.05}$. a) Electron band structure and DOS (DOS values in the range 0 to 16 states/eV/unitcell). b) Phonon band structure, DOS, phonon linewidths (magnification $\times 2$) and Eliashberg function (DOS and $\alpha^2 F$ in the range 0 to 0.12 states/eV/unitcell and 0 to 1.3, respectively). c) Electron and phonon heat capacities. d) Electron-phonon coupling parameter and hot electron thermalisation time.

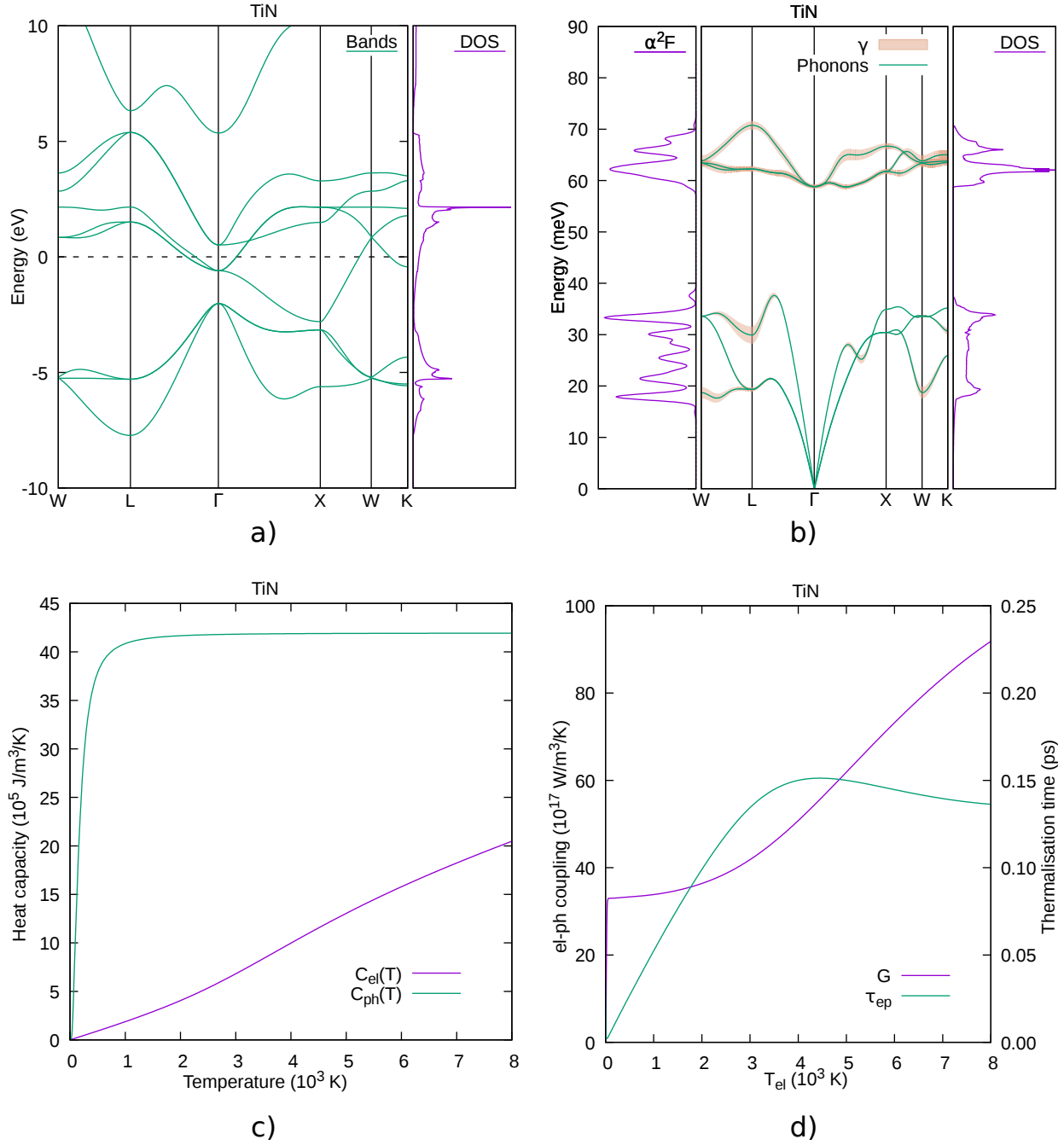


Figure S6: DFT results for TiN. a) Electron band structure and DOS (DOS values in the range 0 to 16 states/eV/unitcell). b) Phonon band structure, DOS, phonon linewidths (magnification $\times 2$) and Eliashberg function (DOS and α^2F in the range 0 to 0.12 states/eV/unitcell and 0 to 1.3, respectively). c) Electron and phonon heat capacities. d) Electron-phonon coupling parameter and hot electron thermalisation time.

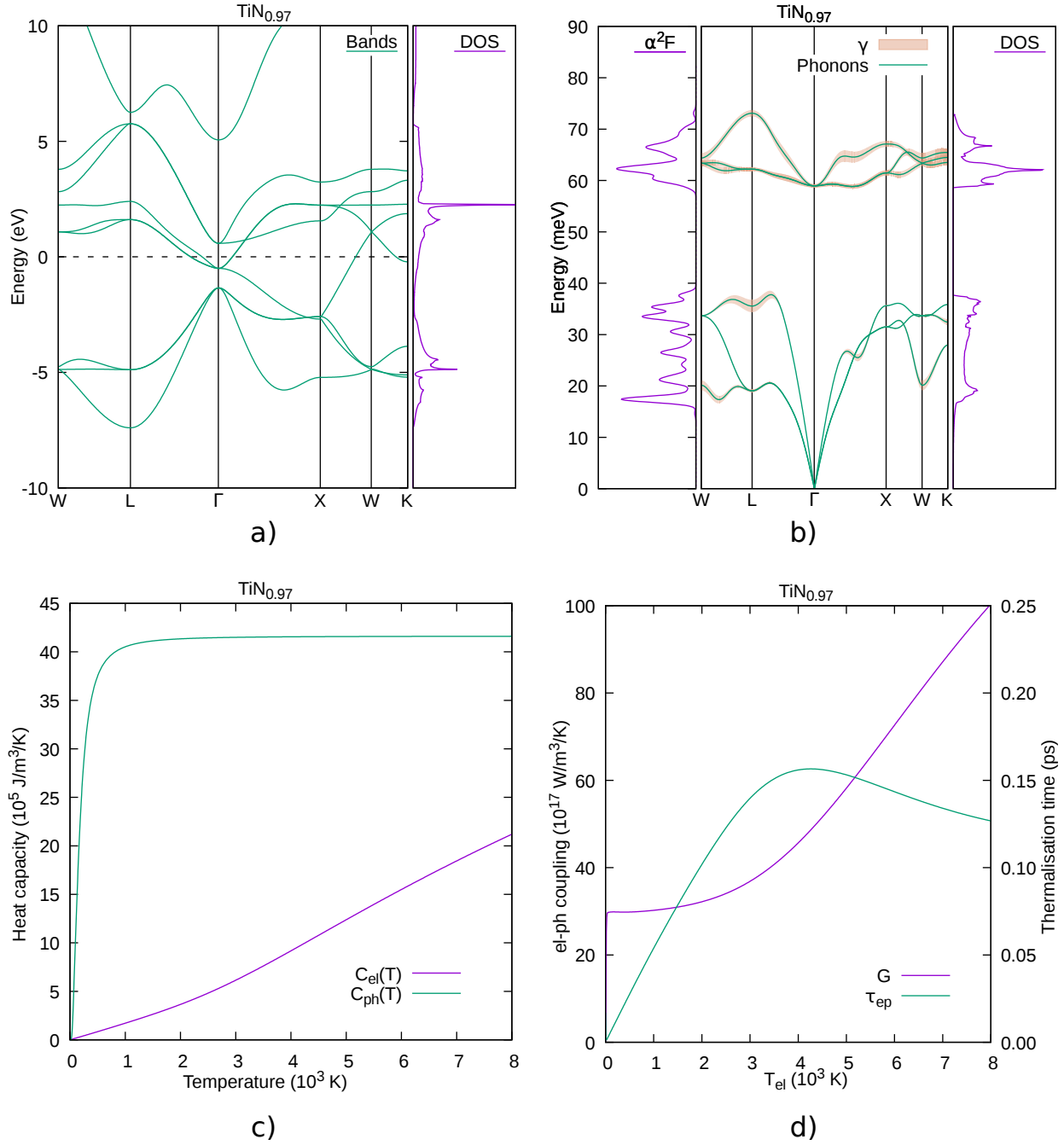


Figure S7: DFT results for $\text{TiN}_{0.97}$. a) Electron band structure and DOS (DOS values in the range 0 to 16 states/eV/unitcell). b) Phonon band structure, DOS, phonon linewidths (magnification $\times 2$) and Eliashberg function (DOS and $\alpha^2 F$ in the range 0 to 0.12 states/eV/unitcell and 0 to 1.3, respectively). c) Electron and phonon heat capacities. d) Electron-phonon coupling parameter and hot electron thermalisation time.

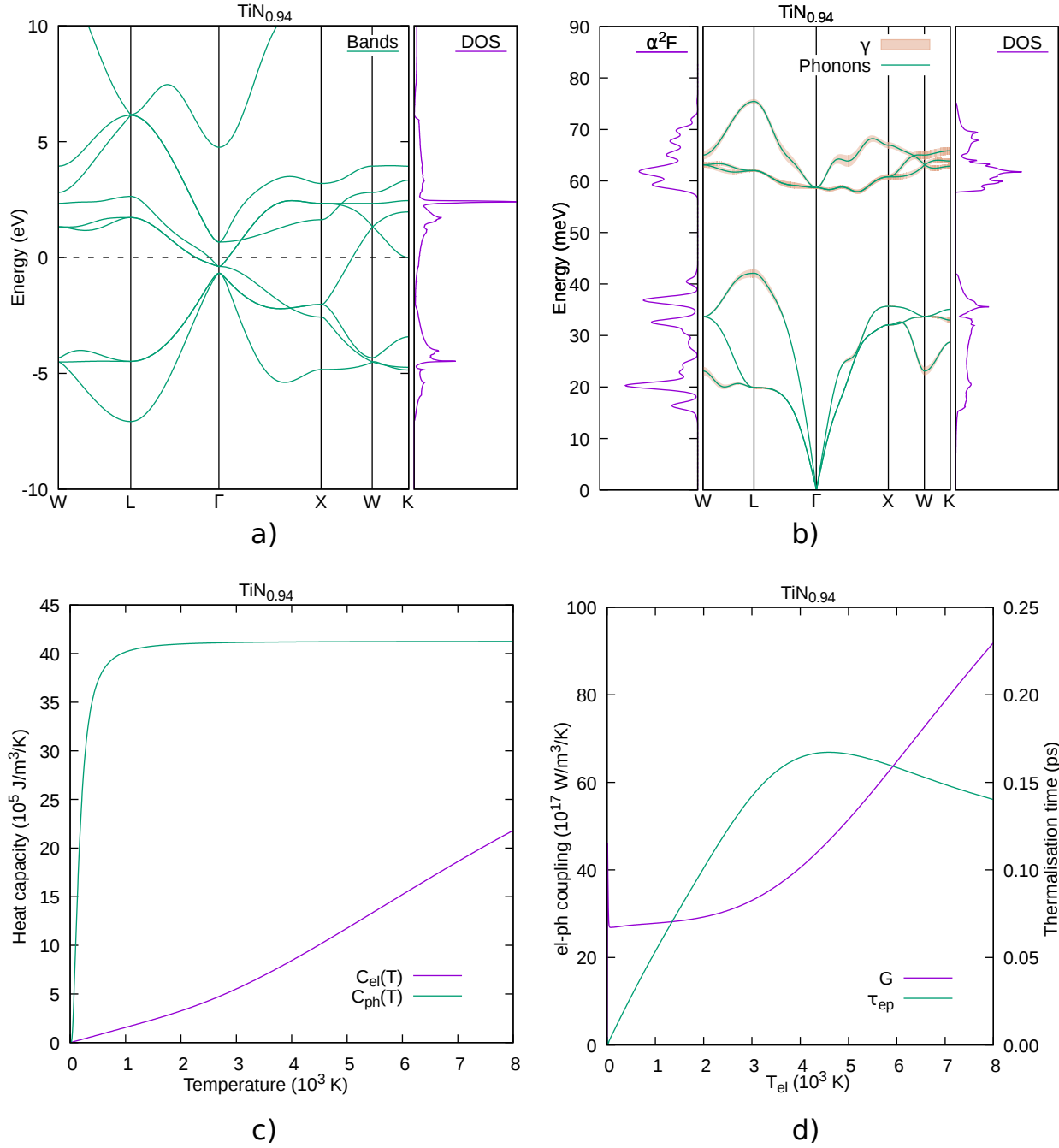


Figure S8: DFT results for $\text{TiN}_{0.94}$. a) Electron band structure and DOS (DOS values in the range 0 to 16 states/eV/unitcell). b) Phonon band structure, DOS, phonon linewidths (magnification $\times 2$) and Eliashberg function (DOS and $\alpha^2 F$ in the range 0 to 0.12 states/eV/unitcell and 0 to 1.3, respectively). c) Electron and phonon heat capacities. d) Electron-phonon coupling parameter and hot electron thermalisation time.

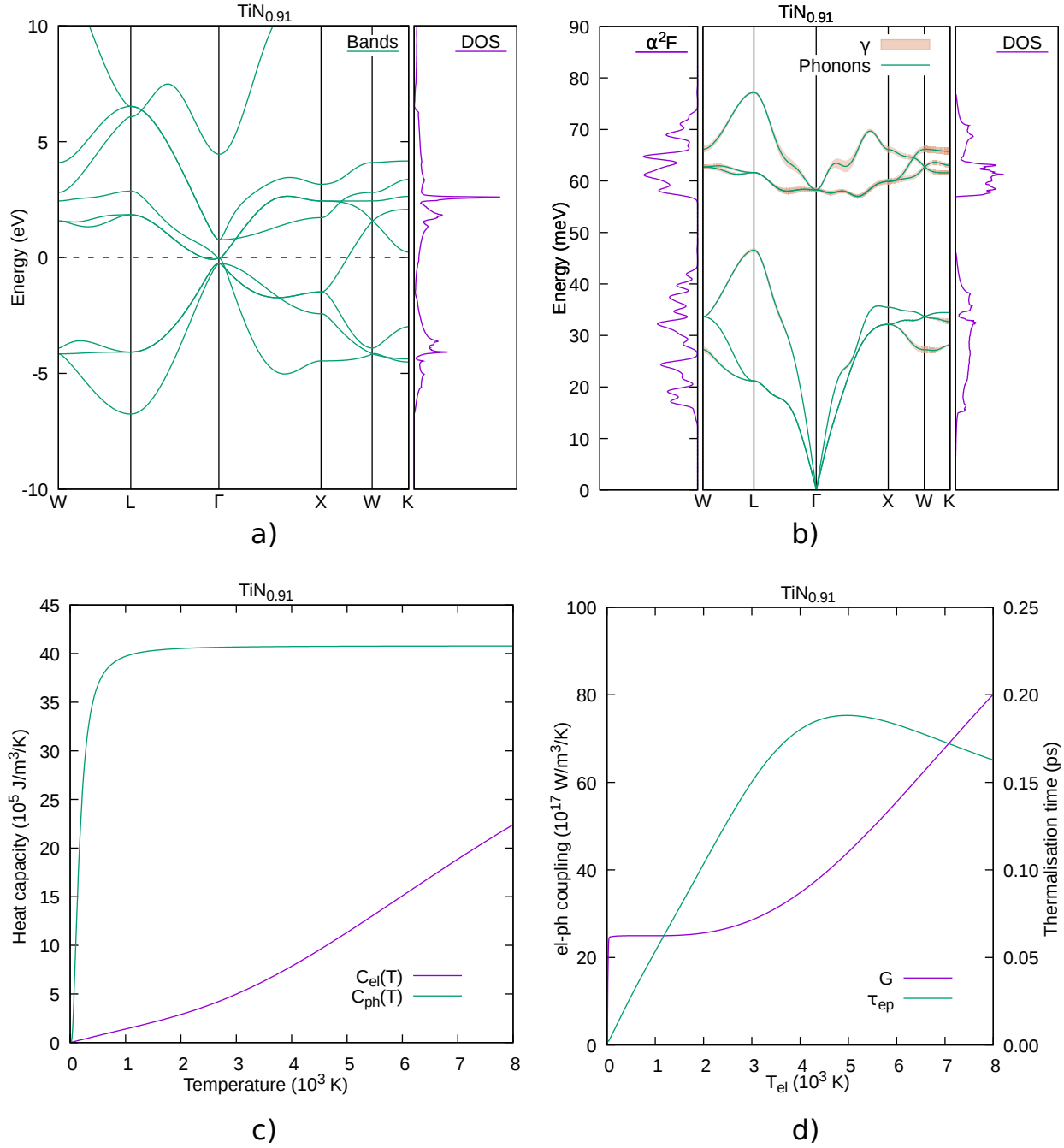


Figure S9: DFT results for $\text{TiN}_{0.91}$. a) Electron band structure and DOS (DOS values in the range 0 to 16 states/eV/unitcell). b) Phonon band structure, DOS, phonon linewidths (magnification $\times 2$) and Eliashberg function (DOS and α^2F in the range 0 to 0.12 states/eV/unitcell and 0 to 1.3, respectively). c) Electron and phonon heat capacities. d) Electron-phonon coupling parameter and hot electron thermalisation time.

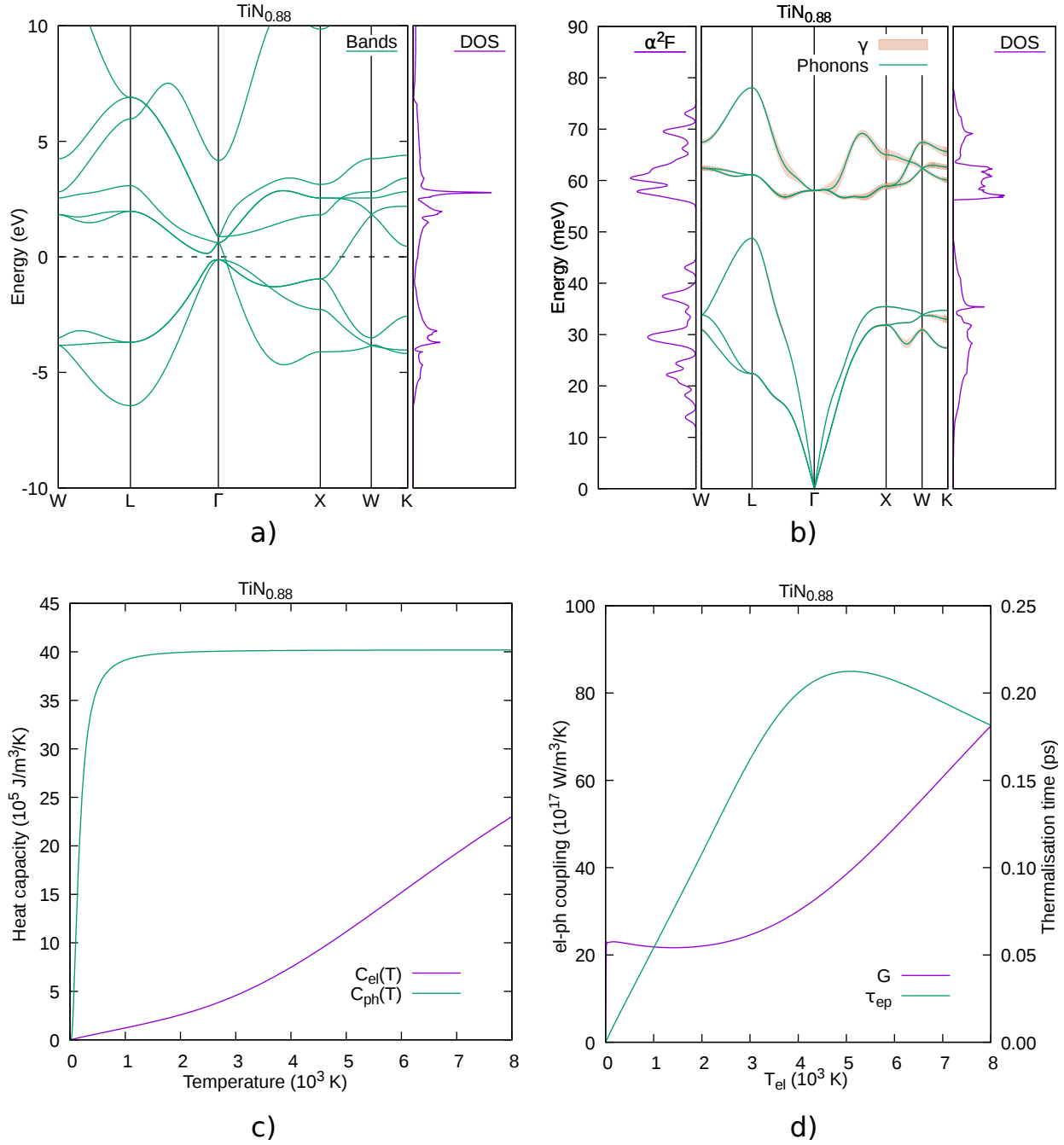


Figure S10: DFT results for $\text{TiN}_{0.88}$. a) Electron band structure and DOS (DOS values in the range 0 to 16 states/eV/unitcell). b) Phonon band structure, DOS, phonon linewidths (magnification $\times 2$) and Eliashberg function (DOS and α^2F in the range 0 to 0.12 states/eV/unitcell and 0 to 1.3, respectively). c) Electron and phonon heat capacities. d) Electron-phonon coupling parameter and hot electron thermalisation time.

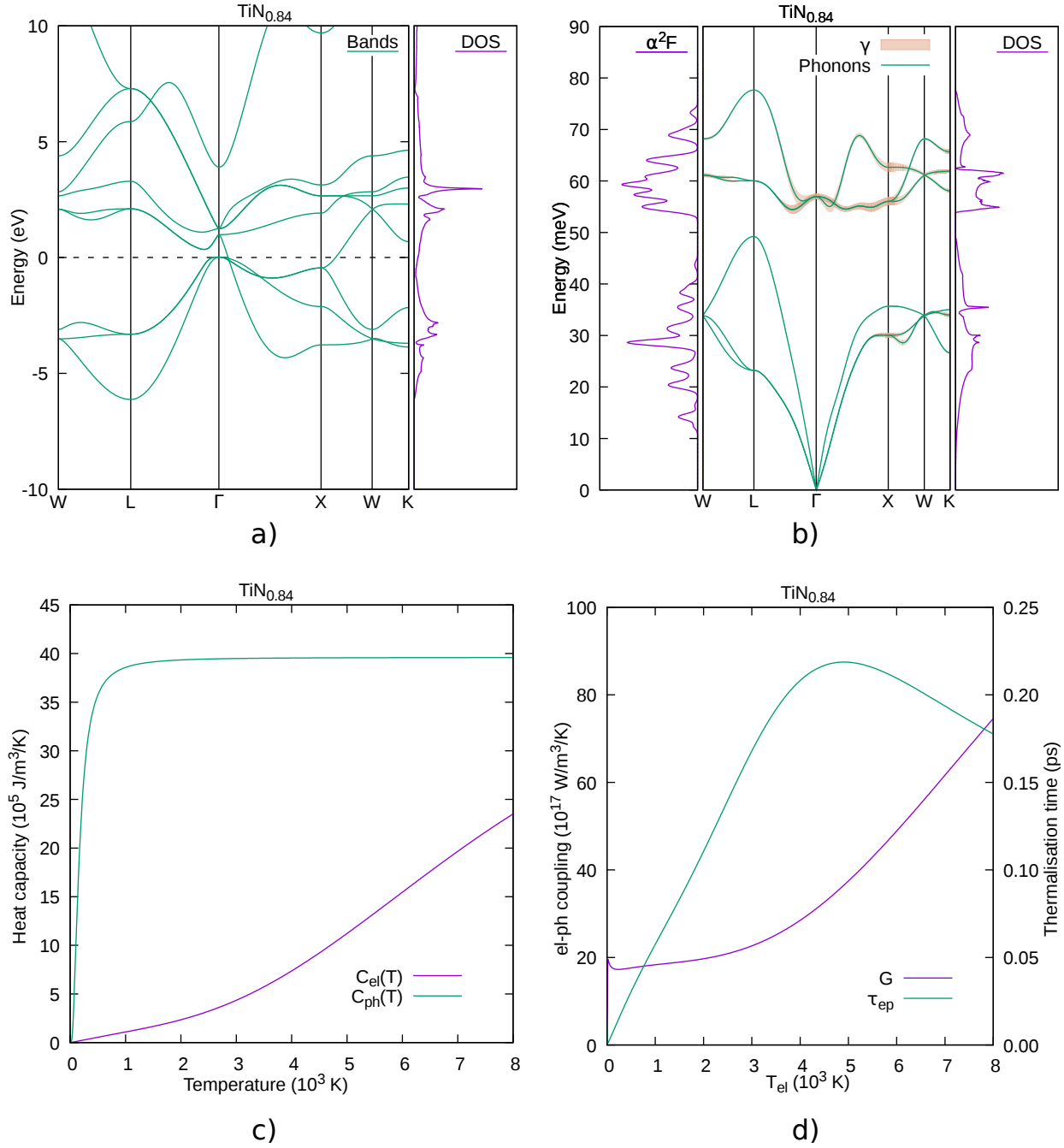


Figure S11: DFT results for $\text{TiN}_{0.84}$. a) Electron band structure and DOS (DOS values in the range 0 to 16 states/eV/unitcell). b) Phonon band structure, DOS, phonon linewidths (magnification $\times 2$) and Eliashberg function (DOS and $\alpha^2 F$ in the range 0 to 0.12 states/eV/unitcell and 0 to 1.3, respectively). c) Electron and phonon heat capacities. d) Electron-phonon coupling parameter and hot electron thermalisation time.