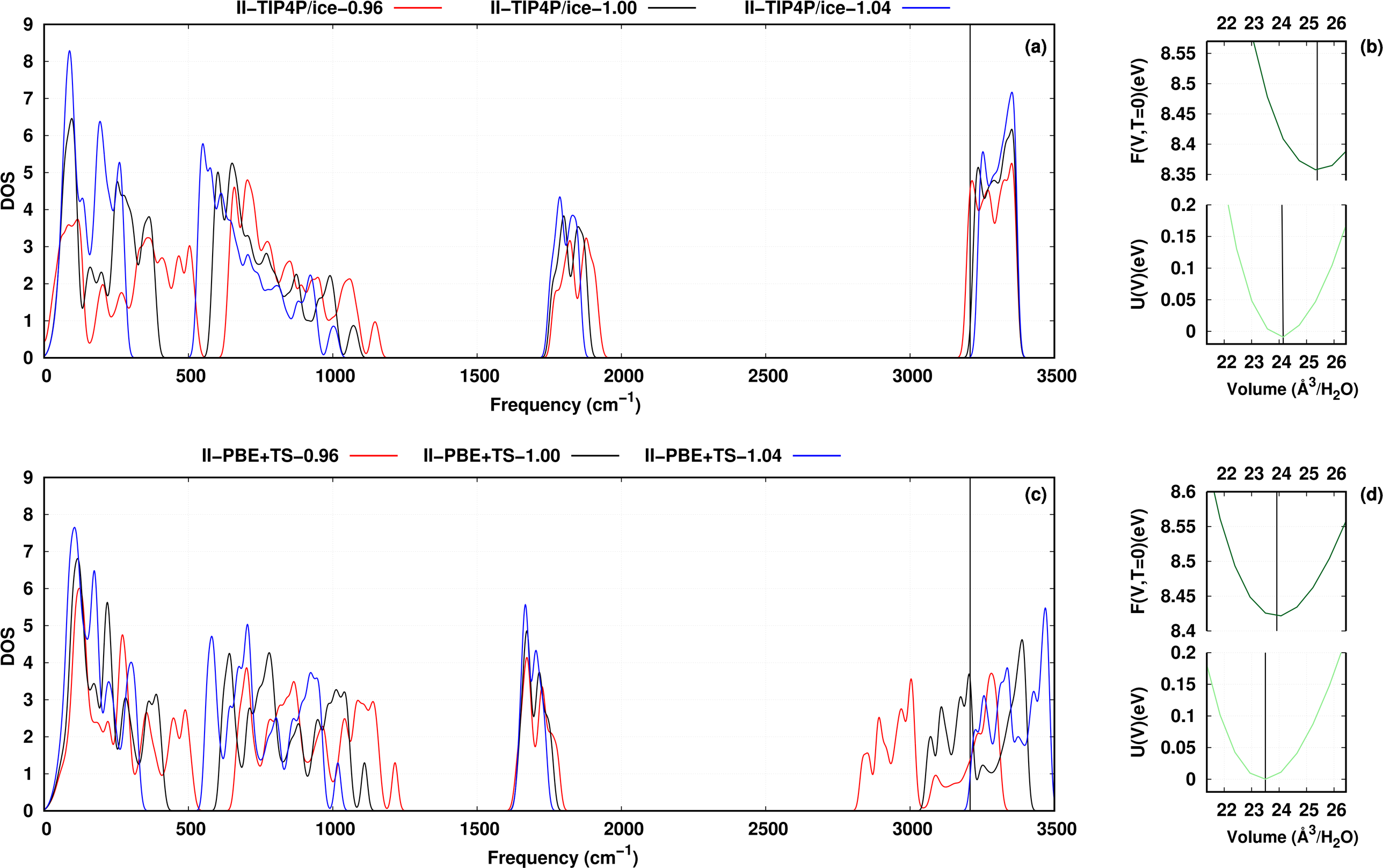
II–TIP4P/ice–0.96
II–TIP4P/ice–1.00
II–TIP4P/ice–1.04
(a)
DOS
Frequency (cm^{-1})
(b)
F(V,T=0)(eV)
U(V)(eV)
Volume (Å^3/H$_2$O)
II–PBE+TS–0.96
II–PBE+TS–1.00
II–PBE+TS–1.04
(c)
DOS
Frequency (cm^{-1})
(d)
F(V,T=0)(eV)
U(V)(eV)
Volume (Å^3/H$_2$O)