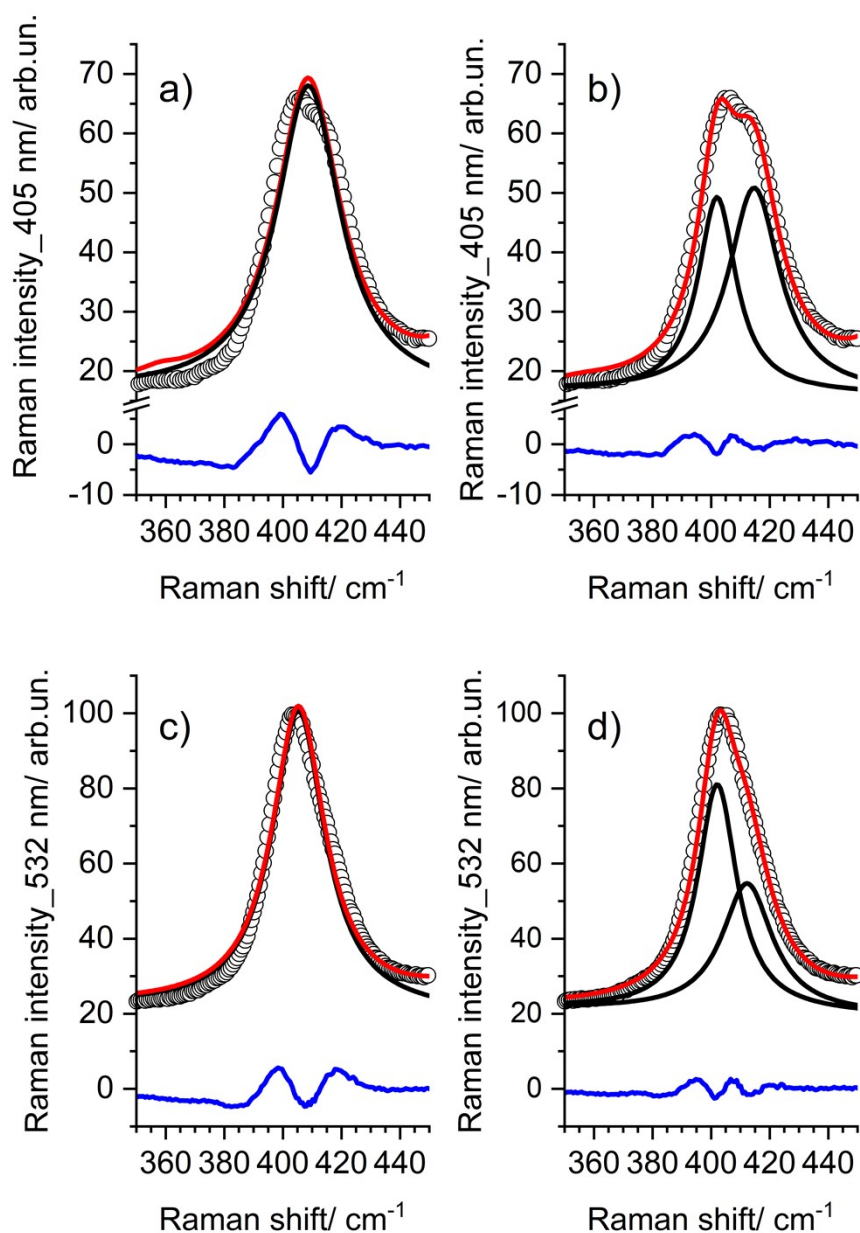
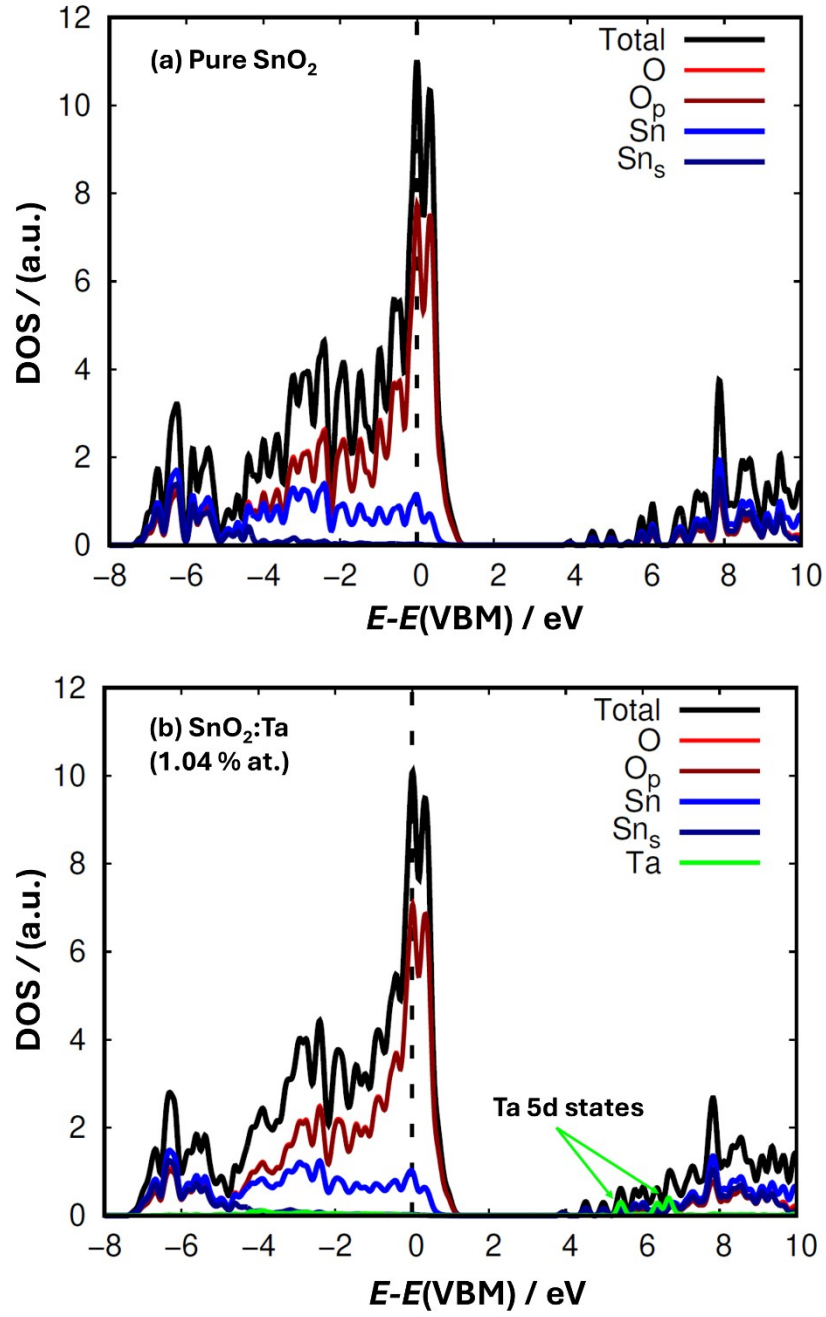


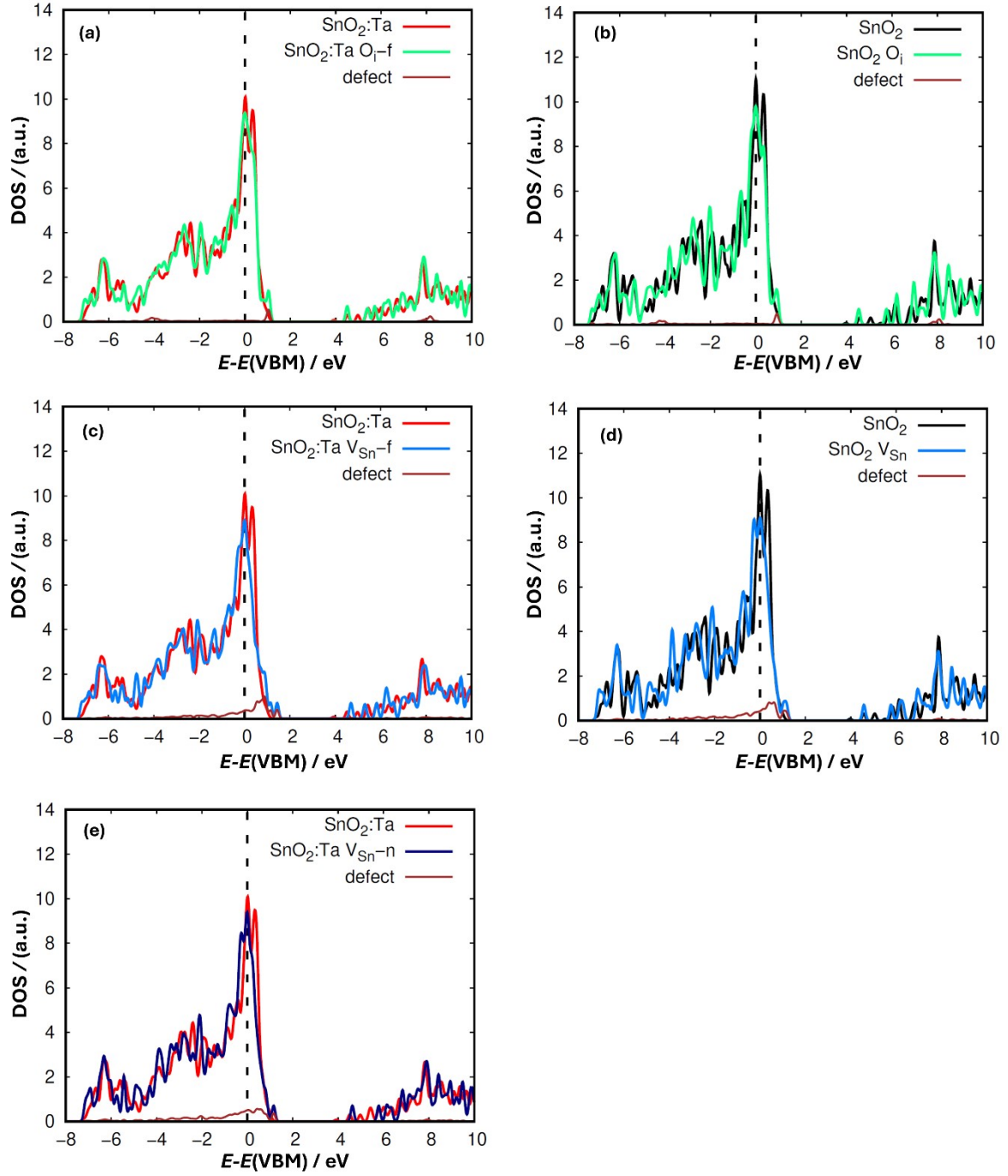
Supporting information



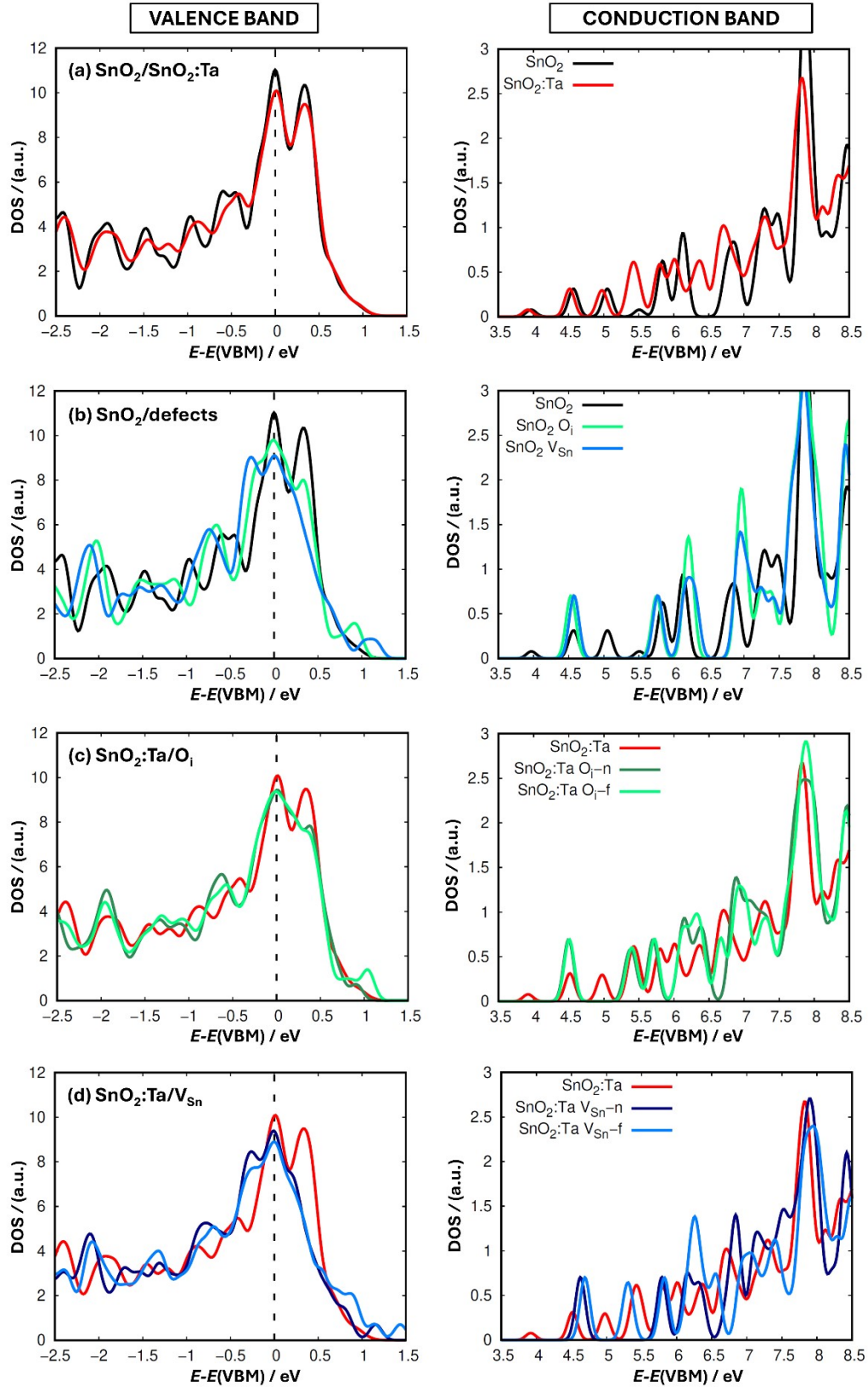
SI 1: Comparison of spectra fits for the D_1 line spectral range measured with two different laser lines. a) one Lorentzian line fit, 405 nm excitation, b) two Lorentzian line fit, 405 nm excitation, c) one Lorentzian line fit, 532 nm excitation, d) two Lorentzian line fit, 532 nm excitation. Measured data (\circ), Cumulative fits (red lines), individual line fits (black lines), fit residue (blue lines).



SI 2: Calculated DOS and PDOS of pure SnO_2 (a) and $\text{SnO}_2:\text{Ta}$ (1.04 % at.) showing the contribution of O 2p-orbitals and Sn s-orbitals.



SI 3: Calculated total and defect density of states of SnO_2 and $\text{SnO}_2:\text{Ta}$ without and with additional point defects. (a) $\text{SnO}_2:\text{Ta}$ with and without O_I -far defect; (b) SnO_2 with and without O_I defect; (c) $\text{SnO}_2:\text{Ta}$ with and without V_{Sn} -far defect; (d) SnO_2 with and without V_{Sn} defect; (e) $\text{SnO}_2:\text{Ta}$ with and without V_{Sn} -close defect.



SI 4: Enlarged VBM and the CBM regions of the density of states of SnO_2 and $\text{SnO}_2:\text{Ta}$ without and with additional point defects.

No.	File name	Model structure	Raman line
1	D1_SnO2-Ta_V-Sn-far	SnO ₂ :Ta_V-Sn-far	D ₁
2	D1_SnO2-Ta_V-Sn-near	SnO ₂ :Ta_V-Sn-near	D ₁
3	D2_SnO2-Ta_V-Sn-near	SnO ₂ :Ta_V-Sn-near	D ₂
4	D2_SnO2-Ta_O-i-far	SnO ₂ :Ta_O-i-far	D ₂
5	L4__SnO2-Ta_O-i-far	SnO ₂ :Ta_O-i-far	L ₄
6	L5__SnO2-Ta_O-i-far	SnO ₂ :Ta_O-i-far	L ₅

SI 5: xyz-files for the visualization of the characteristic vibrational modes responsible for the characteristic Raman lines D₁, D₂, L₄, and L₅ of SnO₂:Ta (1.25 at.% Ta) thin films.