ADVANCED MATERIALS

Supporting Information

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Tailoring Optical Properties in Transparent Highly Conducting Perovskites by Cationic Substitution

Mahdad Mohammadi, Ruiwen Xie, Niloofar Hadaeghi, Aldin Radetinac, Alexey Arzumanov, Philipp Komissinskiy, Hongbin Zhang, and Lambert Alff**

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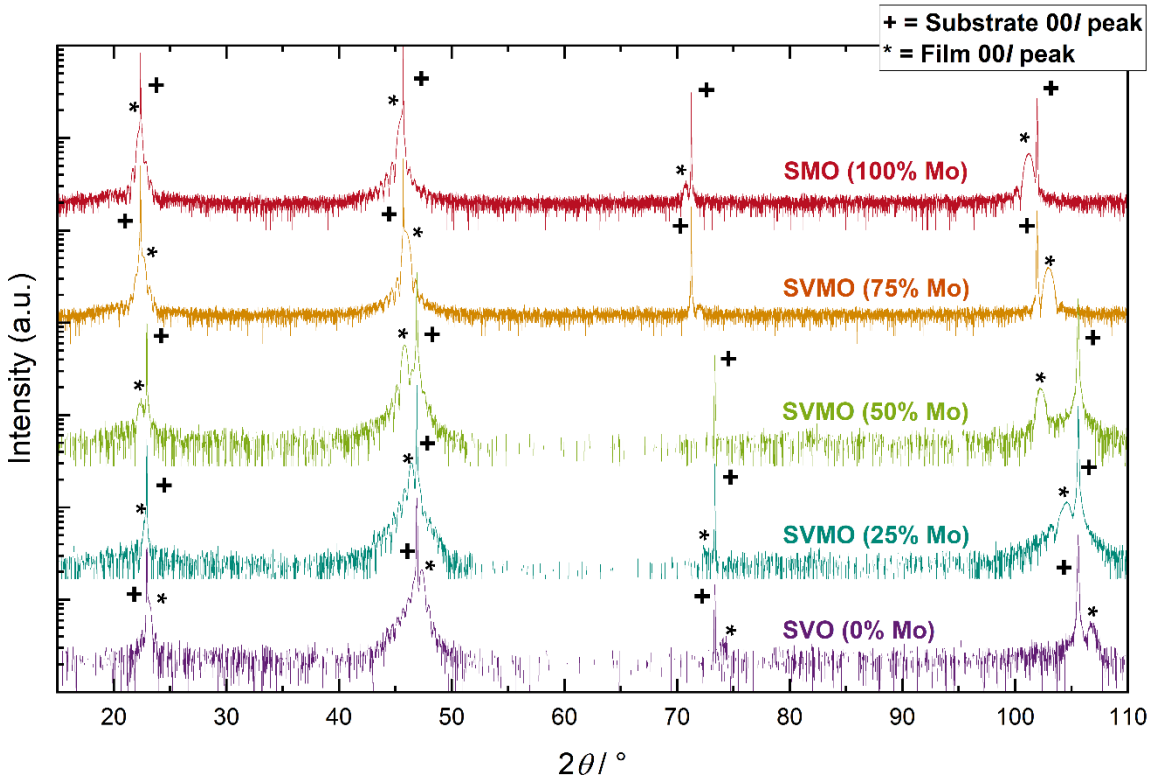

Figure S1. Broad X-ray diffractogram of the mixing series $SrV_{1-x}Mo_xO_3$ (x = 0, 0.25, 0.5, 0.75, 1). The asterisks (crosses) denote the 00*l* diffraction peak of the film (substrate). No additional peaks can be observed, indicating phase purity and no additional orientations.

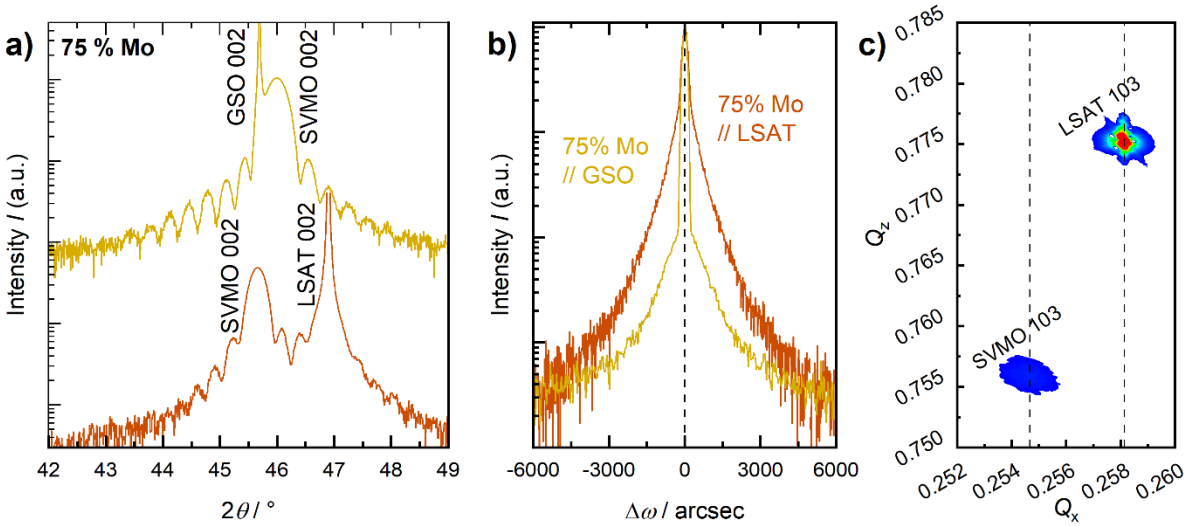

Figure S2. Comparison $SrV_{0.25}Mo_{0.75}O_3$ films grown on $GdScO_3$ and LSAT. a) Close-up scan of the 002 main diffraction peaks of $SrV_{0.25}Mo_{0.75}O_3$ grown on LSAT (lighter brown) and on $GdScO_3$ (darker brown). The stronger Laue oscillations indicate the improved crystalline quality on $GdScO_3$, which is confirmed by the reduced width of the rocking curve (Figure S2 b)). Note that the SVMO films are thicker than in the main manuscript (1000 laser pulses, resulting in 29 nm on $GdScO_3$ and 31.4 nm on LSAT). c) Reciprocal space map around the 103 film peak of $SrV_{0.25}Mo_{0.75}O_3$ grown on LSAT, revealing the relaxed state of the film with respect to the substrate. Compare also to Figure 1 c), where the $SrV_{0.25}Mo_{0.75}O_3$ film grown on $GdScO_3$ is fully strained.

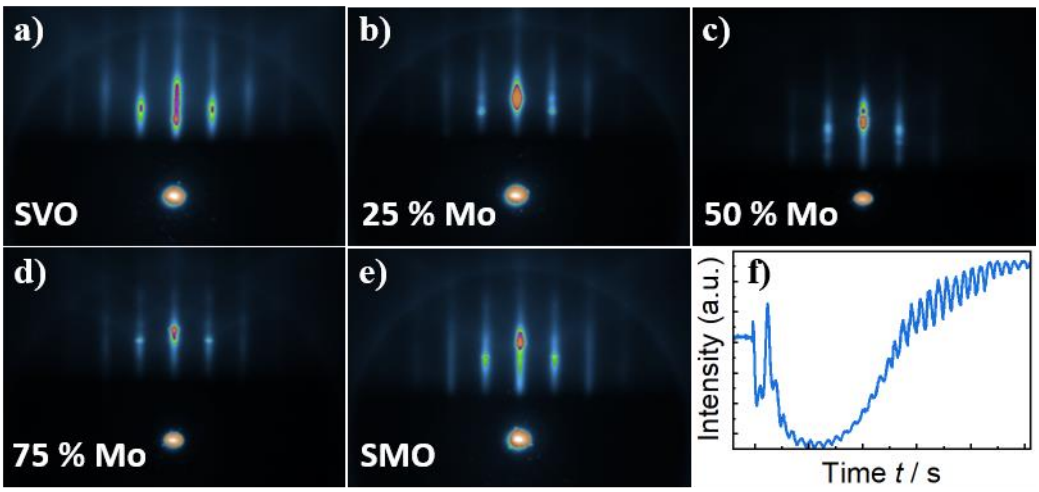

Figure S3. a) – e) Post-growth RHEED pattern of the grown samples in this study. The streaks in the pattern indicate a flat surface and epitaxial growth of the film. f) Cutout of the intensity oscillations of the specular spot during growth, here as an example of $SrV_{0.75}Mo_{0.25}O_3$.

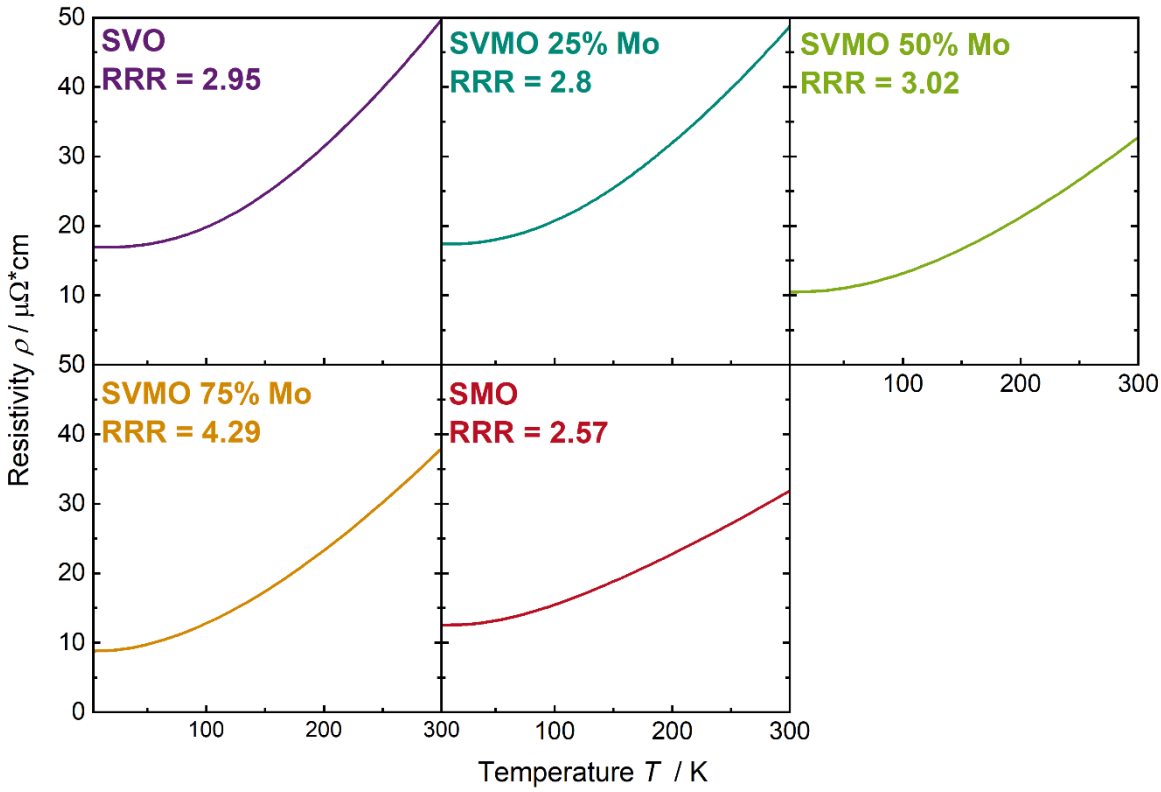

Figure S4. Temperature dependent resistivity measurements of $SrV_{1-x}Mo_xO_3$ (x = 0, 0.25, 0.5, 0.75, 1) between 300 – 4 K. All samples show a positive temperature coefficient and good residual resistivity ratios (RRR).

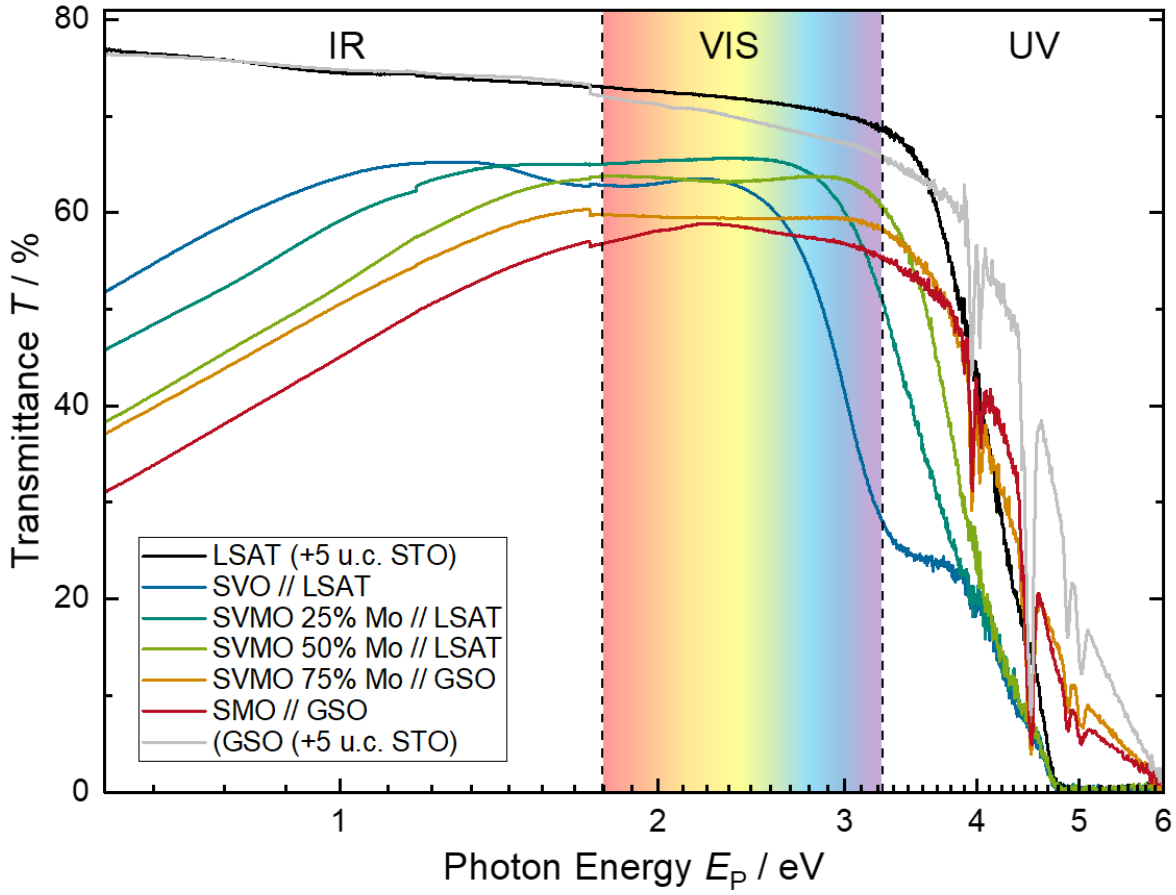

Figure S5: Raw transmittance spectra of the samples (20 nm film+substrate) and transmittance spectra of the substrates covered with a 5 unit cells $SrTiO_3$ (STO) buffer layer.

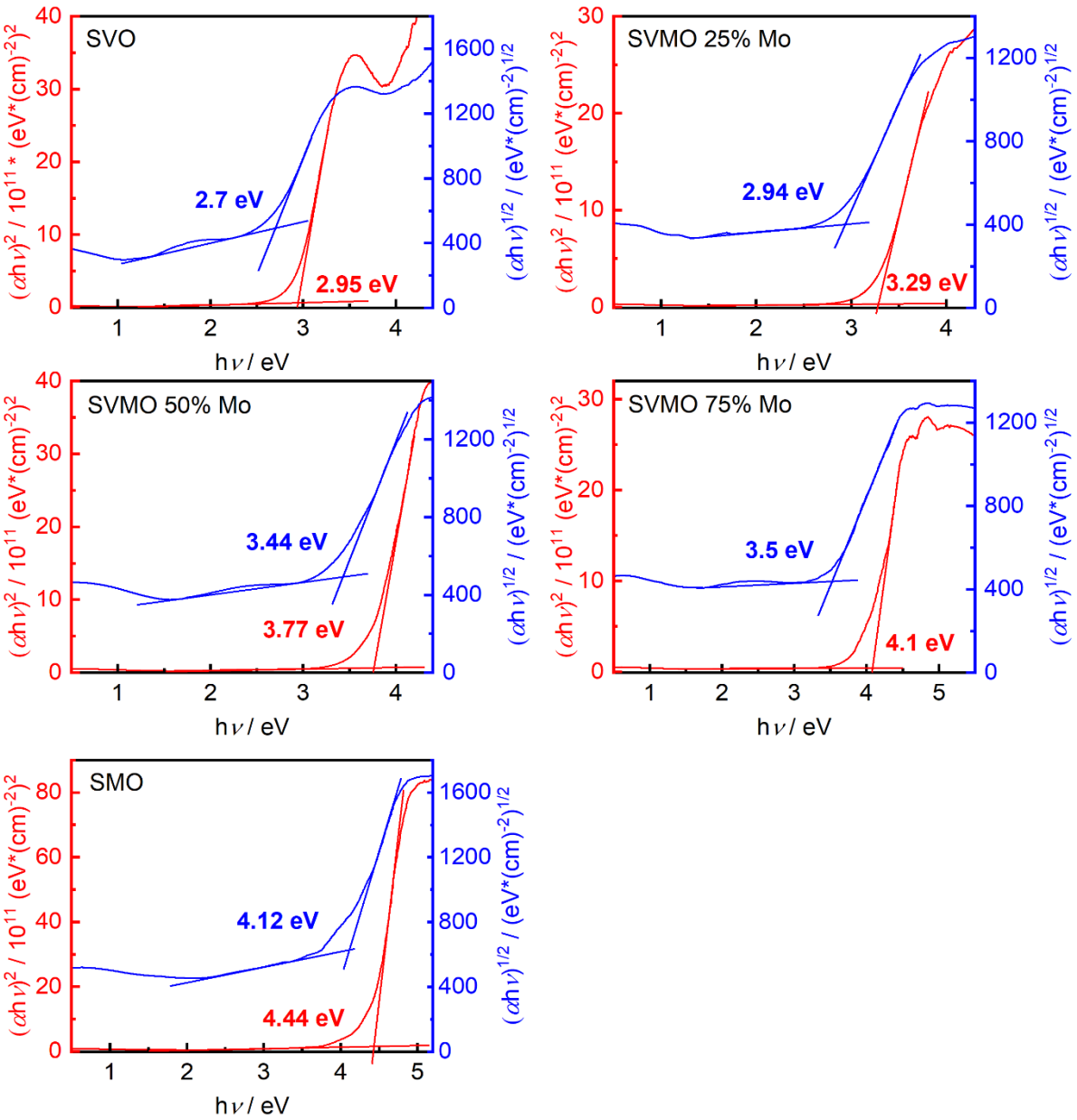

Figure S6. Tauc plots $(\alpha h\nu)^n$ over $h\nu$ for determination of the direct (n = 2) and indirect (n = 1/2) optical transition energies of $SrV_{1-x}Mo_xO_3$ (x = 0, 0.25, 0.5, 0.75, 1)

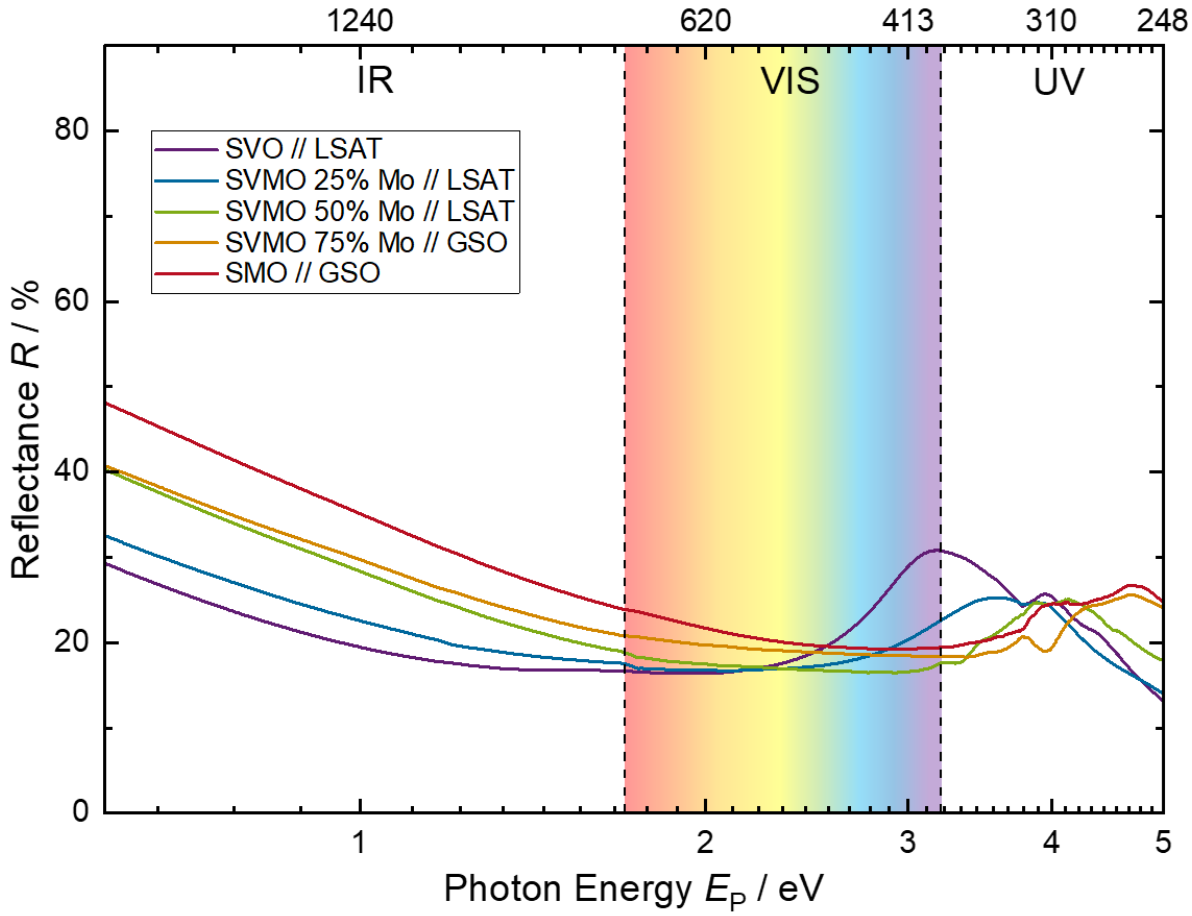

Figure S7. Reflectance spectra of the samples recorded at 6 ° (near-normal) angle of incidence. The spectrum in the IR is governed by the free-carrier reflection in the sample (Drude tail, compare also to the plasma frequency values in Figure 3 b), main manuscript) whereas in the high-energy side of the spectrum the increasing reflection can be assigned to the interband transition of the materials.

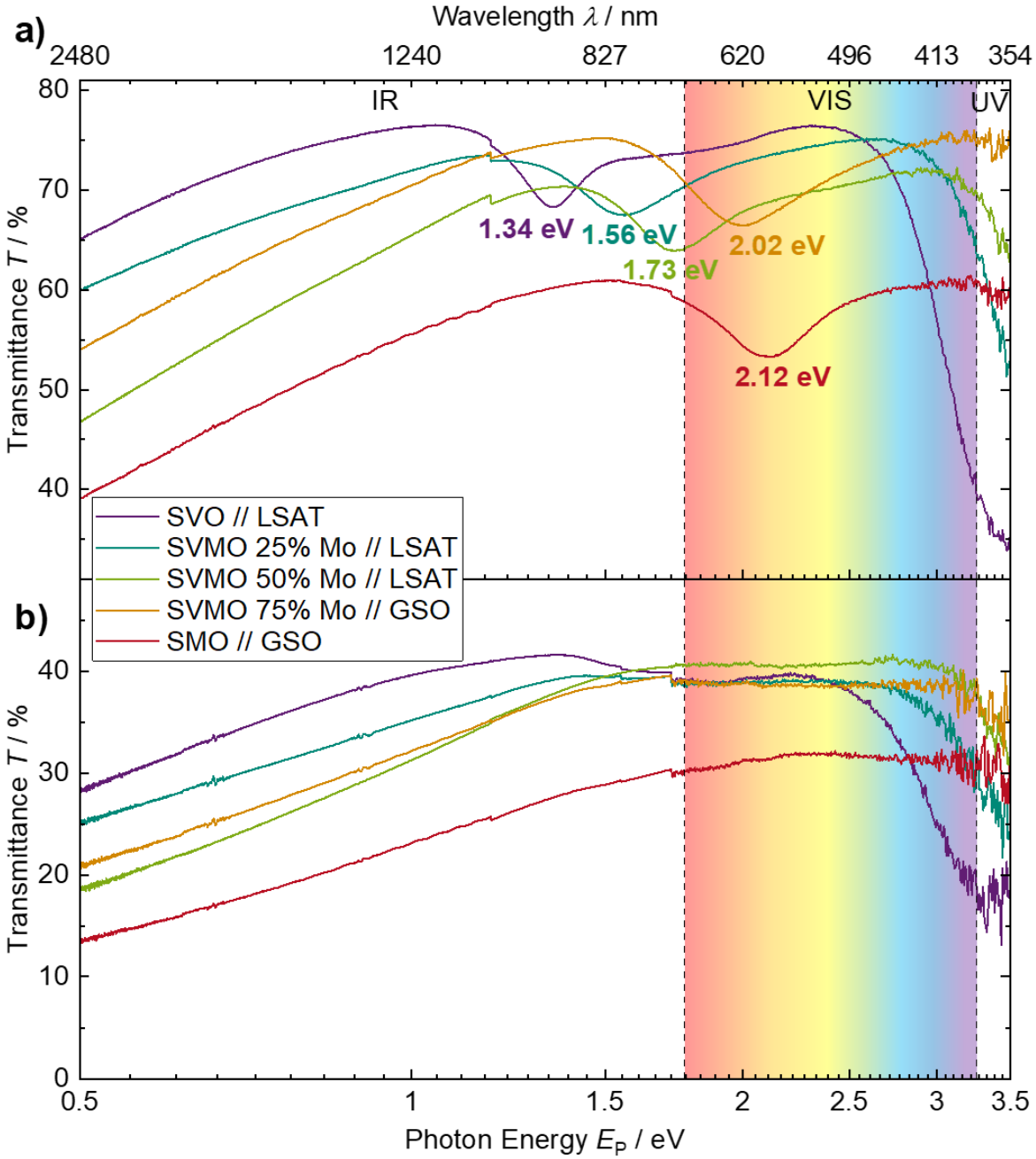

Figure S8. Optical transmittance of a) *p*-polarized and b) *s*-polarized light at an oblique incidence angle of 55 °. The local minima in the transmittance spectra for *p*-polarized light, with a simultaneous absence in the *s*-polarized spectrum, are assigned to the plasmon excitation energy and hence plasma frequency of the material.

Table S1. Haacke FOM for the solid solution series $SrV_{1-x}Mo_xO_3$ at different wavelengths.

	Φ_{TC} @ 320 nm / 10^{-3}	Φ_{TC} @ 550 nm / 10^{-3}	Φ_{TC} @ 720 nm / 10^{-3}	Φ_{TC} average / 10^{-3}
$SrVO_3$	$4.49*10^{-3}$	7.51	6.88	3.34
25 % Mo	1.38	11.06	8.53	9.51
50 % Mo	10.22	11.30	10.89	11.88
75 % Mo	15.55	9.21	7.08	10.36
100 % Mo	9.69	8.95	4.61	8.49

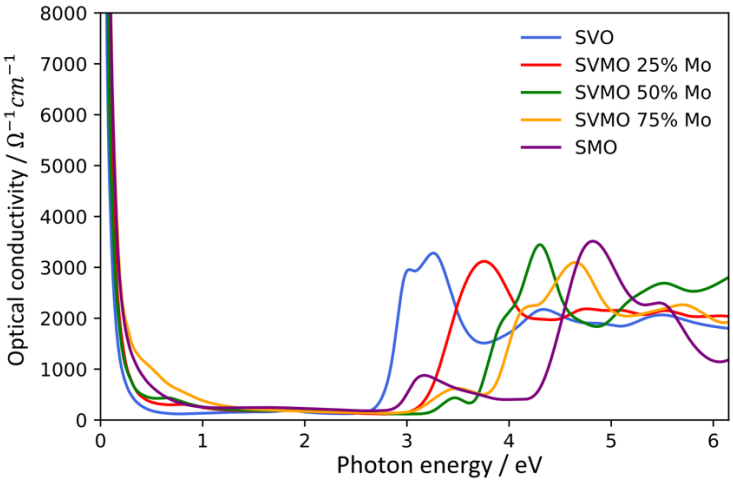

Figure S9. Optical conductivities of $Sr(V_{1-x}Mo_x)O_3$ with x = 0, 0.25, 0.50, 0.75, 1, respectively, calculated using DFT + DMFT approach.

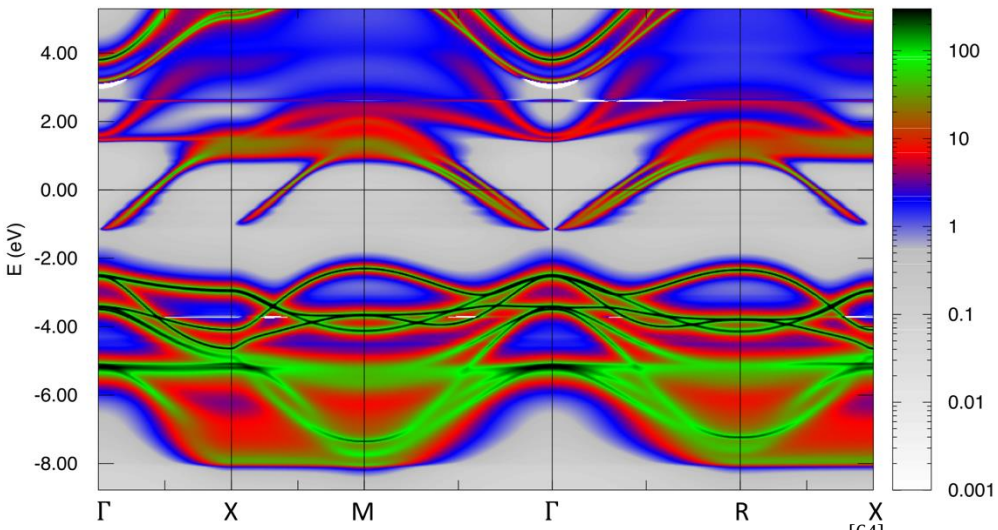

Figure S10. Calculated band structure of $Sr(V_{0.5}Mo_{0.5})O_3$ using SPR-KKR[64] in which the Mo doping is simulated as completely random based on the coherent potential approximation. The color code is for the band weight.

Supporting References

[64] Ebert, H., A. Vernes, J. Banhart, *Solid state commun.* **1997**, *104*, 243.