Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Electronic Supplementary Information

Pressure-Driven Multiple Optoelectronic Evolution in $CsMoO_3(IO_3)$ with Dual Functional $[MoO_6]$ and $[IO_3]$ Groups

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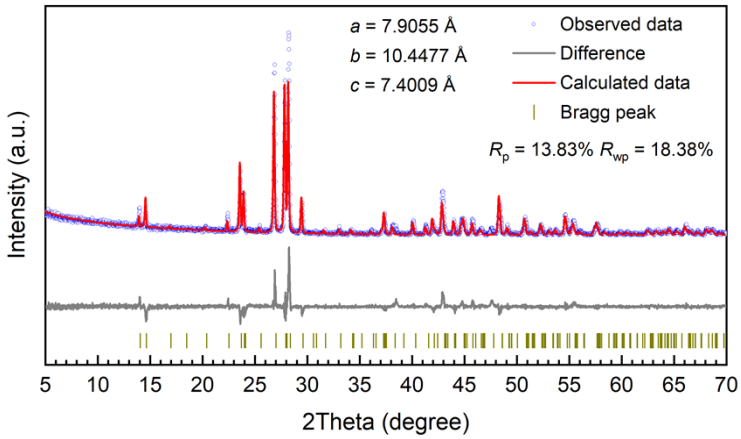

Figure S1. *Lebail* refinement of $CsMoO_3(IO_3)$ at ambient condition with the space group of $Pna2_1$, cell parameters a = 7.9055 Å, b = 10.4477 Å, c = 7.4009 Å.

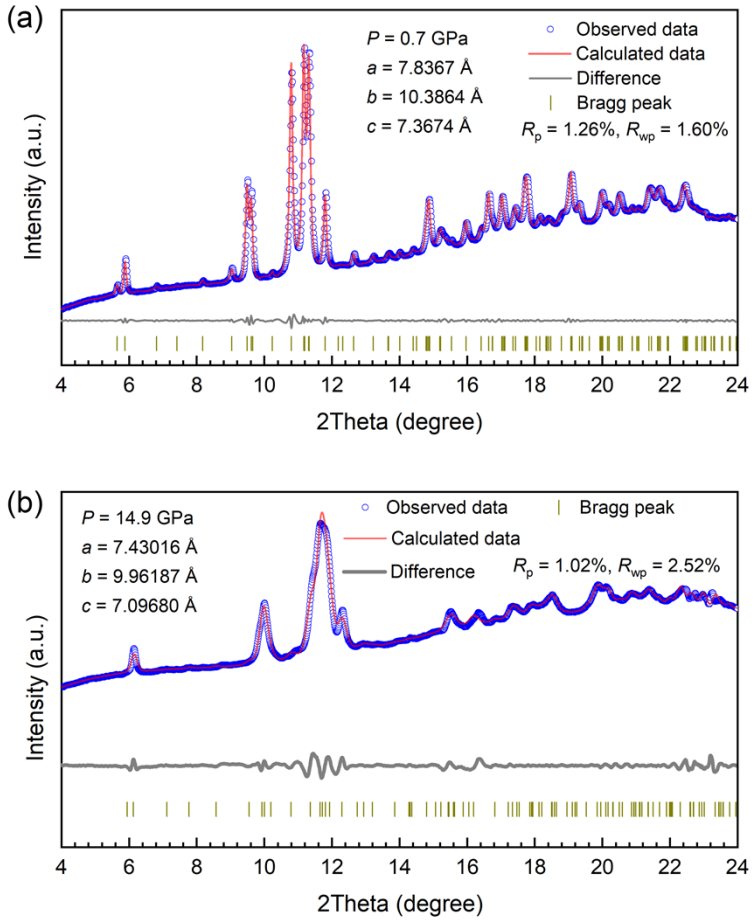

Figure S2. *Lebail* refinement of $CsMoO_3(IO_3)$ at 0.7 GPa, and 14.9 GPa.

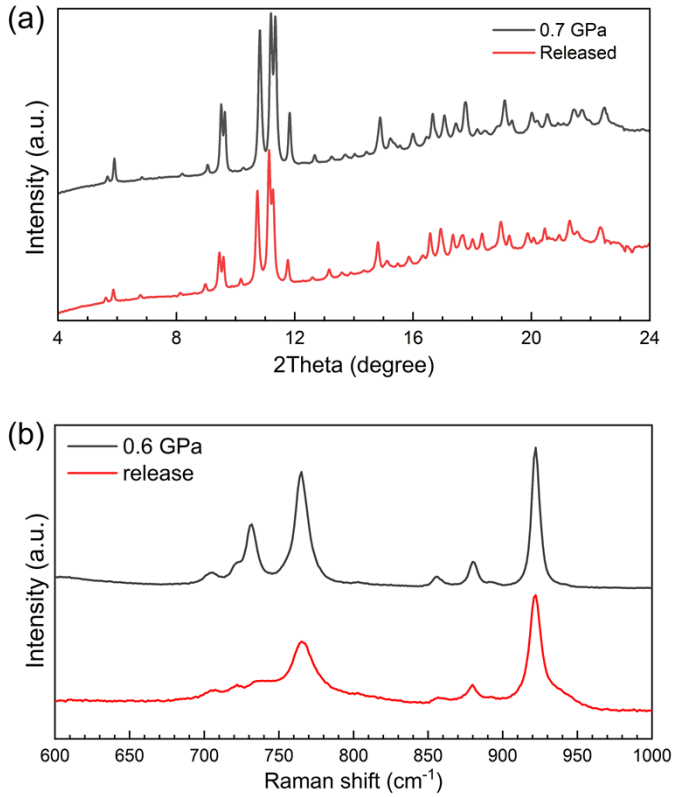

Figure S3. (a) The XRD patterns of the released sample and the sample at 0.7 GPa. (b) The Raman spectra the released sample and the sample at 0.6 GPa in the region of 600-1000 cm^{-1}.

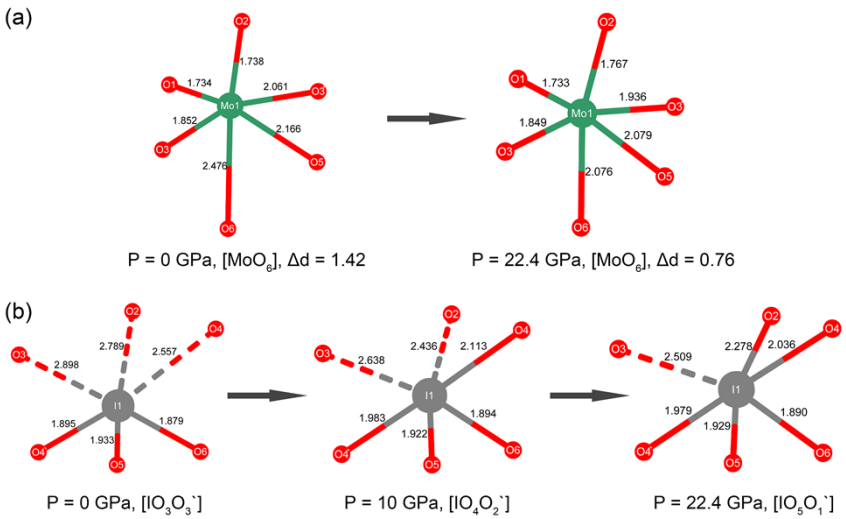

Figure S4. Models of the $[MoO_6]$ and $[IO_3]$ groups obtained by geometry optimization at selective pressures.

Table S1. The contribution of dual functional groups to the optoelectronic properties.

	Piezochromism	SHG transformation	Enhancement of photocurrent switching ratio
$[MoO_6]$ group	√	√	√
$[IO_3]$ group	×	√	√