Electronic Supplementary Material (ESI) for RSC Advances.
This journal is © The Royal Society of Chemistry 2017

In the case of perovskite materials, the following parameters can be used as reliable polyhedra deformation indicators [i-ii]:

Distortion index ***D***:

$$D = \frac{1}{n}\sum_{i=1}^{n}\frac{\left|l_i - l_{av}\right|}{l_{av}}$$

where l_i is the distance from the central atom to the i^{th} coordinating atom, and l_{av} is the average bond length.

Quadratic elongation <λ>:

$$<\lambda>=\frac{1}{n}\sum_{i=1}^{n}\left(\frac{l_i}{l_0}\right)^2$$

where l_0 is a bond length in a regular polyhedron of the same volume and thus <λ> is a dimensionless parameter, a quantitative measure of polyhedral distortion independent of its effective size.

Bond angle variance σ^2:

$$\sigma^2 = \frac{1}{m-1}\sum_{i=1}^{m}\left(\phi_i - \phi_0\right)^2$$

where m is a number of bond angles, $\boldsymbol{\phi_i}$ is $\boldsymbol{i}^{th}$ bond angle and $\boldsymbol{\phi_0}$ = 90° (ideal bond angle in regular octahedron).

Effective coordination number ***ECoN***:

$$ECoN = \sum_i w_i; \qquad w_i = \exp\left[1-\left(\frac{l_i}{l_{av}}\right)^6\right]; \qquad l_{av} = \frac{\sum_i l_i \exp[1-(l_i/l_{\min})^6]}{\sum_i \exp[1-(l_i/l_{\min})^6]}$$

where w_i is i^{th} bond weight, l_{av} is weighted average bond length and l_{min} is the smallest bond length in the coordination octahedron.

[i] W. H. Baur, *Acta Crystallogr., Sect. B: Struct. Sci.*, 1974, **30**, 1195.
[ii] R. Hoppe, *Z. Kristallogr.*, 1979, **150,** 23.

Table S1. Effective masses of electrons and holes (scaled by m_0; the values in parentheses

correspond to spin-up, spin-down and average effective masses).

$SrTiO_3$ ***h*** (up / dn / average)		***e*** (up / dn / average)		
$R \rightarrow \Gamma$	**$R \rightarrow X$**	**$\Gamma \rightarrow M$**	**$\Gamma \rightarrow R$**	**$\Gamma \rightarrow X$**
(-0.607 / -0.607 / -0.607)	(-0.828 / -0.828 / -0.828)	(0.38 / 0.38 / 0.38)	(0.628 / 0.628 / 0.628)	(0.352 / 0.352 / 0.352)
(-0.608 / -0.608 / -0.608)	(-1.015 / -1.015 / -1.015)	(0.504 / 0.504 / 0.504)	(0.522 / 0.522 / 0.522)	(0.352 / 0.352 / 0.352)
(-1.511 / -1.511 / -1.511)	(-2.756 / -2.756 / -2.756)	(0.66 / 0.66 / 0.66)	(0.499 / 0.499 / 0.499)	(5.464 / 5.464 / 5.464)
$SrTi_{0.98}Nb_{0.02}O_3$				
$Z \rightarrow \Gamma$	**$Z \rightarrow R$**	**$\Gamma \rightarrow M$**	**$\Gamma \rightarrow Z$**	**$\Gamma \rightarrow X$**
(-0.905 / -0.905 / -0.905)	(-0.799 / -0.799 / -0.799)	(0.384 / 0.384 / 0.384)	(0.387 / 0.387 / 0.387)	(0.344 / 0.344 / 0.344)
(-0.938 / -0.937 / -0.938)	(-0.799 / -0.799 / -0.799)	(0.618 / 0.618 / 0.618)	(0.387 / 0.387 / 0.387)	(0.346 / 0.346 / 0.346)
(-6.341 / -6.442 / -6.391)	(-14.414 / -15.266 / -14.84)	(0.859 / 0.859 / 0.859)	(2.219 / 2.32 / 2.27)	(5.511 / 5.621 / 5.566)
$SrTi_{0.97}Nb_{0.03}O_3$				
$M \rightarrow \Gamma$	**$M \rightarrow X$**	**$\Gamma \rightarrow M$**	**$\Gamma \rightarrow Z$**	**$\Gamma \rightarrow X$**
(-0.943 / -0.943 / -0.943)	(-0.823 / -0.823 / -0.823)	(0.405 / 0.405 / 0.405)	(0.372 / 0.372 / 0.372)	(0.365 / 0.365 / 0.365)
(-1.049 / -1.051 / -1.05)	(-0.826 / -0.826 / -0.826)	(0.608 / 0.609 / 0.609)	(0.372 / 0.372 / 0.372)	(0.365 / 0.372 / 0.369)
(-2.777 / -2.798 / -2.788)	(-15.599 / -12.871 / -14.235)	(0.737 / 0.752 / 0.745)	(4.629 / 4.979 / 4.804)	(5.324 / 4.208 / 4.766)