Erratum: Photoelastic and elastic properties of the fluorite structure materials, LiF, and Si [Phys. Rev. B 68, 155120 (2003)]

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All the corrections presented in this Erratum stem from our misunderstanding of the definition of ζ. The reference and table numbers in the following refer to the original paper.

On page 5, col. 1, the sentence beginning "When $\zeta=1$," is to be replaced with the following:

For the traceless [111] strain, the condition $\zeta=1$ characterizes bond bending, i.e., preservation of both the [111] bond length as well as the inequivalent $[\bar{1}11]$, $[1\bar{1}1]$, and $[11\bar{1}]$ bonds.[15,36]

On page 5, col. 2, the entire discussion from "Regrettably" to the end of the paragraph is retracted. Instead:

The present calculation agrees with two previous LDA calculations[30,31] for the value of ζ. In addition, Christensen[38] has argued for $0.40\leqslant\zeta\leqslant0.60$ using a semiempirical argument based on a linear muffin tin orbital calculation.

On page 6, col. 2, $\zeta=0.81$ is to be replaced with $\zeta=0.54$.

On page 7, Fig. 3 caption: $\zeta=0.81,0.73$ is to be replaced with $\zeta=0.54,0.49$. The clause "which is representative of the experimental data presented in Table IV" is retracted.

On page 9, col. 1, "a change in ζ of 0.2–0.3" is to be replaced with "a change in ζ of 0.1–0.2."

On page 9, Fig. 13 caption and figure: "$\zeta=0.6,0.4725,0.345$" is to be replaced with "$\zeta=0.4,0.315,0.23$."

On page 9, Fig. 14 caption and figure: "$\zeta=0.623,0.525,0.435,0.405$" is to be replaced with "$\zeta=0.42,0.35,0.29,0.27$."

On page 10, Fig. 15 caption and figure: "$\zeta=0.668,0.540,0.381,0.315,0.285$" is to be replaced with "$\zeta=0.45,0.36,0.25,0.21,0.19$."

On page 11, col. 2, the paragraph beginning "We believe…" is also retracted.

On page 11, add to Ref. 14: This work used a nonstandard definition of ζ based an a particular nonvolume-conserving strain. The values of ζ presented in Ref. 14 have been multiplied by $3/2$ to correspond to Kleinman's definition when used in the present paper.

Table IV is to be amended as shown.

We thank Manuel Cardona for alerting us to the correct definition of ζ and to the errors in the original discussion.

TABLE IV. Internal strain parameter ζ, a pure number, for silicon and fluorite structure compounds. The quantity Ω of Ref. 40 equals ζ.

			ζ
Si	Expt.	Ref. 63	0.75 ± 0.07
	Expt.	Ref. 64	0.65 ± 0.04
	Expt.	Ref. 45	0.72 ± 0.04
	Expt.	Ref. 46	0.74 ± 0.04
	LDA	Ref. 30	0.53
	LDA	Ref. 31	0.545
	LDA	present	0.54
CaF_2	LDA force field	present	0.31
		Ref. 40	0.216
$Ca_{0.75}Sr_{0.25}F_2$	LDA	present	0.35
$Ca_{0.50}Sr_{0.50}F_2$	LDA	present	0.38
$Ca_{0.25}Sr_{0.75}F_2$	LDA	present	0.40
SrF_2	LDA force field	present	0.41
		Ref. 40	0.266
BaF_2	LDA force field	present	0.45
		Ref. 40	0.377

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