Erratum: Short- and medium-range structure of amorphous zircon from molecular dynamics simulations [Phys. Rev. B 74, 214204 (2006)]

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We correct an error in the presentation of the potential model parameters. The correct potential parameters are given in Table I.

We also note that it has been shown in previous molecular dynamics simulations that a slight increase in the A parameter (to 2029.2204 eV) for the O-O interaction led to simulated silicate glass structures in better agreement with neutron diffraction experimental data in terms of the Si-O distances.[1–3] This modification has also been used in the study of low density (LD) amorphous zircon using micro-canonical ensembles (NVT). The amorphous zircon structures obtained using the original and modified parameters are very similar except that the modified parameters give slightly larger Si-O bond length (1.60 vs. 1.59 Å), in agreement with previous findings.[1–3]

TABLE I. Buckingham potential parameters

Pairs	A (eV)	ρ (Å)	C (eV.Å^6)
$Si^{2.4}$-$O^{-1.2}$	13702.905	0.193817	54.681
$O^{-1.2}$-$O^{-1.2}$	1844.7458	0.343645	192.58
$Zr^{2.4}$-$O^{-1.2}$	17943.394	0.226627	127.65

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