Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for:

Anomalous elastic properties in Stishovite

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1. Selecting the Optimal Functional

As may be observed from Figure S1, for all the functionals tested, the systems seem to converge at the same energy cut-off and the same *k* sampling grid, 1000 eV with a 4x4x6 mesh. In Table S1 it may be observed that even though the methods studied seem to converge at the same level, the correlation with experimental data is best obtained when using the LDA functional.

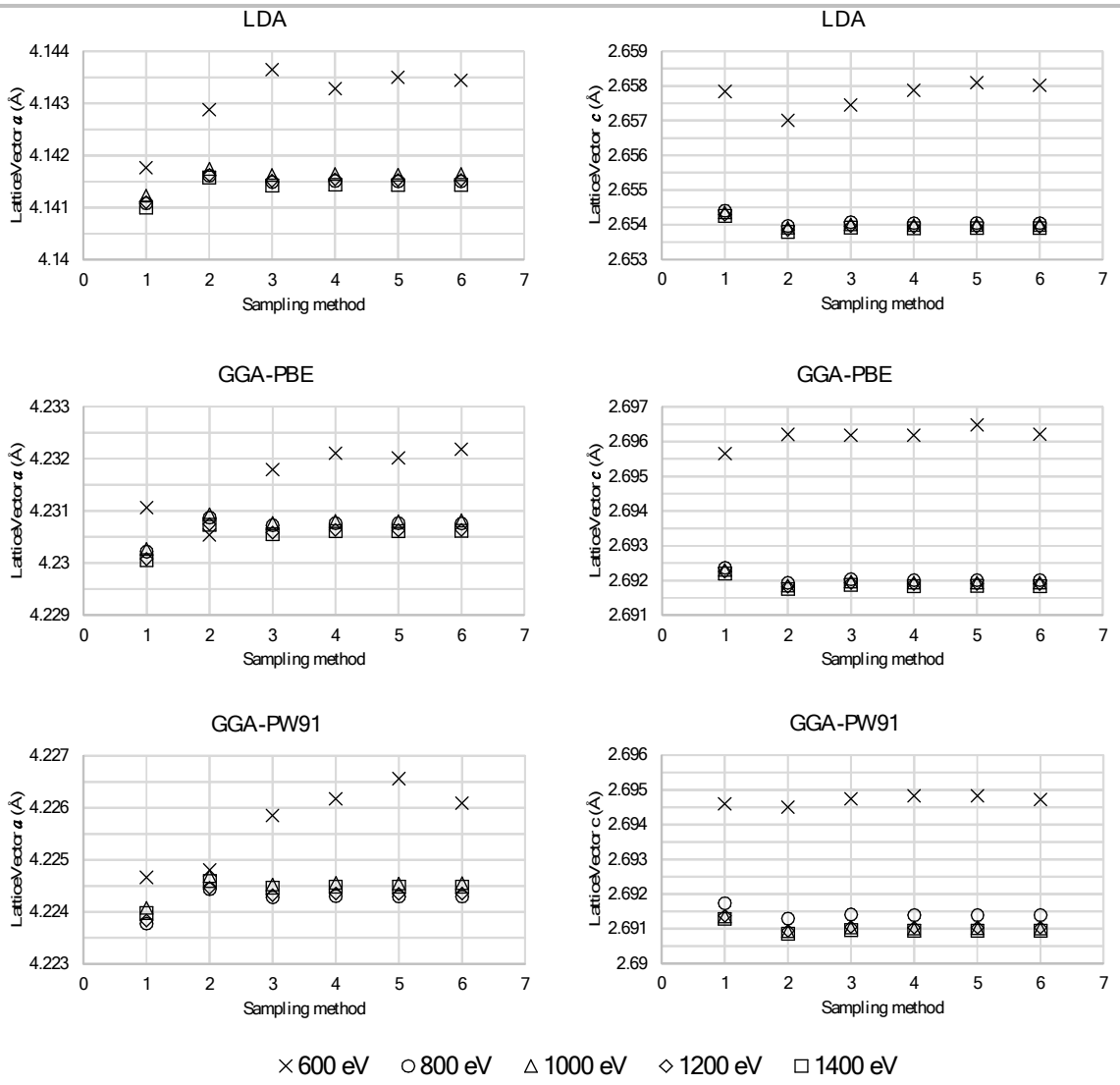

Figure S1: Convergence testing of the three functional studied (LDA, GGA-PBE and GGA-PW91). Convergence testing was carried out with respect to sampling mesh as well as the cut off energy. Sampling methods represent the Monkhorst-Pack k-point grid as follows; 1: 3x3x5, 2: 4x4x6, 3: 5x5x7, 4: 6x6x8, 5: 7x7x9, 6: 8x8x10.

Table S1: Comparison of the calculated lattice parameters and the experimental lattice parameters as presented by Ross (1990)

	a (Å)	***b*** (Å)	***c*** (Å)
LDA	-0.038	-0.038	-0.016
GGA-PBE	0.051	0.051	0.022
GGA-PW91	0.044	0.044	0.021

2. Convergence Criteria

The convergence criteria used are listed in Table S2.

Table S2: The convergence criteria used for the geometry optimizations using the BFGS minimizer.

Energy	$5x10^{-6}$ eV/atom
Maximum Force	0.01 eV/ Å
Maximum Stress	0.02 GPa
Maximum Displacement	$5x10^{-4}$ Å

3. X-ray Diffraction Spectra

X-ray diffraction spectra for the structure of stishovite minimized at 0, 15 and 30 GPa were obtained using the Reflex module in Materials Studio. The powder diffraction application was applied using settings as published elsewhere.[S1] It is evident that there is a constant shift of the major peak on increasing the applied pressure, indicating the measured structural changes.

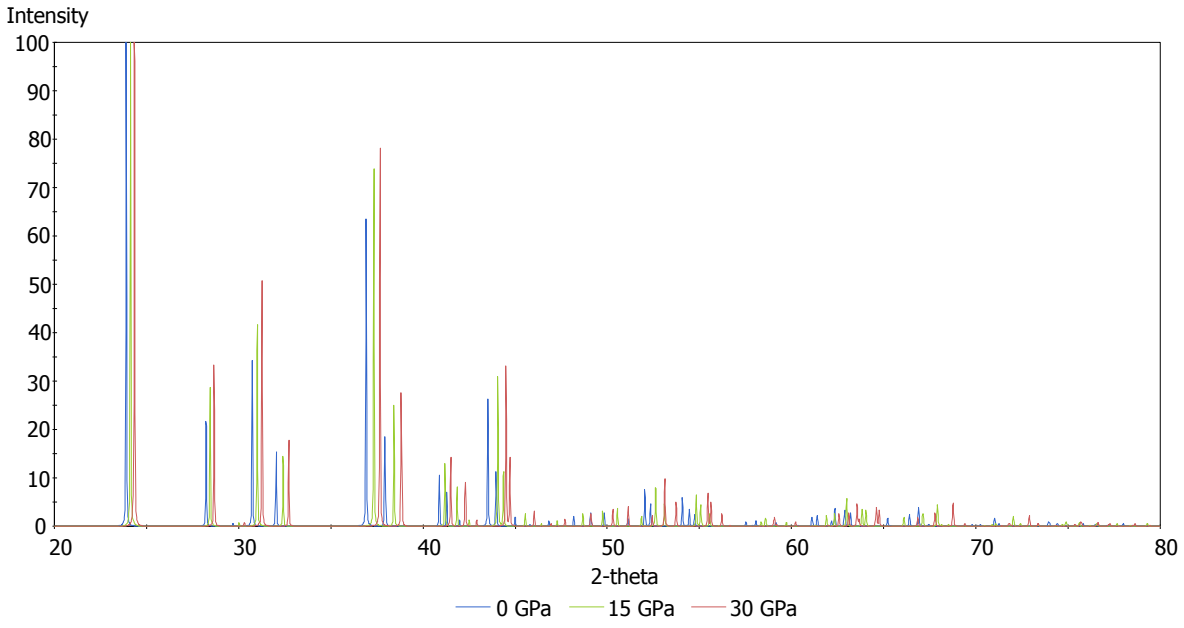

Figure S2: X-ray diffraction spectra obtained for the structure of stishovite minimized at 0, 15 and 30 GPa.

4. Reference

S1 N. L. Ross, J. F. Shu, R. M. Hazen and T. Gasparik, *Am. Mineral.*, 1990, **75**, 739.