Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting information for:

An extensive theoretical survey of low-density allotropy in silicon

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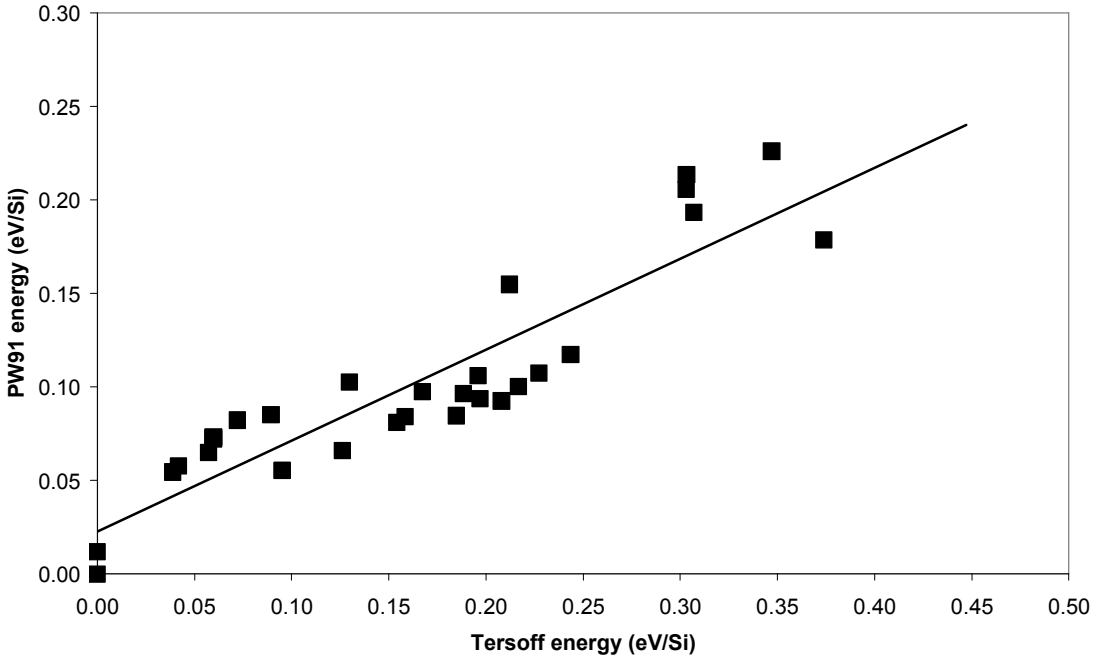

Fig. S1 Tersoff potential calculated energies with respect to diamond for a range of silicon structures plotted against their PW91 calculated counterparts. The range of structures considered included the 5-6 clathrates, the structures taken from Conesa (including *ngs*) and the structures based on known zeolites. The R^2 value of the linear fit obtained (line shown) is 0.82.

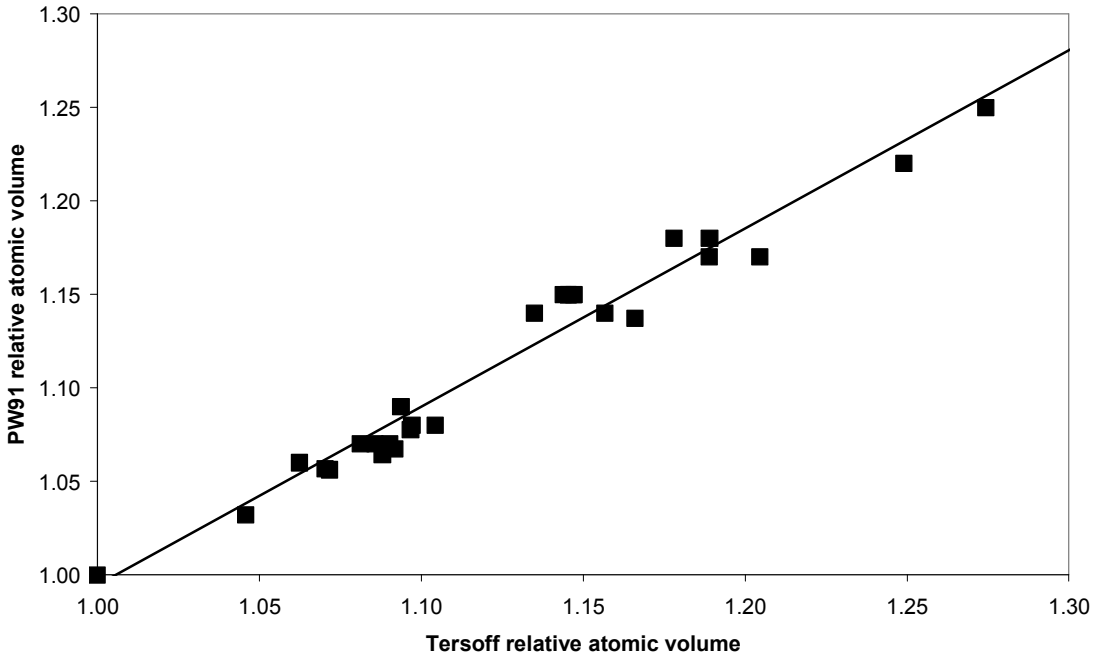

Fig. S2 Tersoff potential calculated relative atomic volumes with respect to diamond for a range of silicon structures plotted against their PW91 calculated counterparts. The range of structures considered is the same as for Fig. S1. The R^2 value of the linear fit obtained (line shown) is 0.96.