Supplementary information for:

Structure and dynamics in amorphous tellurium and Te\textsubscript{n} clusters: A density functional study

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Abstract

Figures 1 and 2 show the notation used for isomers of S\textsubscript{n}\textsuperscript{1} and in the present work on Te\textsubscript{n} clusters. Figure 3 compares pair distribution functions $g(r)$ and structure factors $S(Q)$ (TPSS, PBE, and BLYP approximations at 720 K) with high energy XRD data measured at 763 K (Ref. 2).


Figures
FIG. 1: [Supplementary Figure 1] Isomers of $S_n$ ($n = 3 - 10$). From Ref. 1.

FIG. 2: [Supplementary Figure 2]
FIG. 3: [Supplementary Figure 3] (a) Pair distribution functions $g(r)$ and (b) Structure factors $S(Q)$ calculated for the TPSS, PBE, and BLYP approximations at 720 K. Also show are high energy XRD data measured at 763 K (Ref. 2).