Supplementary Material for:

Density functional study of structure and dynamics in liquid antimony and Sb$_n$ clusters

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The Supplementary Material provides additional results of the above simulations. Figure SF1 shows plots of the ratio of dynamical structure factors $S(q, E)$ to the static structure factor $S(q)$ for selected values of $q$ at 600 K, 900 K, and 1300 K. Figures SF2–SF5 show structures of Sb$_5$ to Sb$_{14}$, and Fig. SF6 shows the vibrational densities of states for selected stable isomers of Sb$_n$.

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Figure 1: [Fig. SF1] (following) Plots of ratio $S(q, E)/S(q)$ for Sb with selected values of $q$ at 600 K, 900 K, 1300 K.
600 K

$S(q, E)/S(q)$

Energy [meV]

$\text{DF/MD } q = 0.237 \, \AA^{-1}$

$\text{DF/MD } q = 0.685 \, \AA^{-1}$

$\text{DF/MD } q = 0.867 \, \AA^{-1}$

$\text{DF/MD } q = 1.043 \, \AA^{-1}$

$\text{DF/MD } q = 1.184 \, \AA^{-1}$
$600 \text{ K}$

![Graph showing the relationship between energy and intensity of different q values.](image)

- **DF/MD q=1.988 \text{ \AA}^{-1}**
- **DF/MD q=2.042 \text{ \AA}^{-1}**
- **DF/MD q=2.072 \text{ \AA}^{-1}**
- **DF/MD q=2.124 \text{ \AA}^{-1}**
- **DF/MD q=2.17 \text{ \AA}^{-1}**

The y-axis represents $S(q,E)/S(q)$ and the x-axis represents energy in [meV].
900 K

$S(q,E)/S(q)$

Energy [meV]

-20 -15 -10 -5 0 5 10 15 20

DF/MD $q=0.929 \, \text{Å}^{-1}$

DF/MD $q=1.019 \, \text{Å}^{-1}$

DF/MD $q=1.069 \, \text{Å}^{-1}$

DF/MD $q=1.111 \, \text{Å}^{-1}$

DF/MD $q=1.172 \, \text{Å}^{-1}$
Energy [meV]

S(q,E)/S(q)
Figure 2: [Fig. SF2] Isomers of Sb$_5$, Sb$_6$, and Sb$_7$. (a) denotes the most stable isomer, (b) the next highest in energy.
Figure 3: [Fig. SF3] Isomers of Sb$_8$, (a) to (h) in order of decreasing stability. The weak “bonds” between the tetrahedra in Sb$_8$(b) are 4.23 Å long, in Sb$_8$(c) 3.99 Å.
Figure 4: [Fig. SF4] Isomers of Sb$_9$, Sb$_{10}$, and Sb$_{11}$. (a) denotes the most stable isomer, (b) the next highest in energy.
Figure 5: [Fig. SF5] Isomers of Sb$_{12}$, Sb$_{13}$, and Sb$_{14}$. (a) denotes the most stable isomer, (b) the next highest in energy.
Figure 6: [Fig. SF6] Vibration densities of states for selected stable isomers of Sb$_n$. Frequencies are broadened by a Gaussian function of width 1 cm$^{-1}$. 