**GeSe2 Density Check**

**May 12, 2019**

**From QM simulation data (qm\_1100\_GeSe2)**

Total number of atoms: 384 (128 Ge + 256 Se)

Lattice constant: 23x23x19.32

The number density: 384/(23\*23\*19.32) = 0.0375 (Å-3) = 3.751022 (cm-3)

**From MLMD simulation data (GeSe2-1100K)**

Total number of atoms: 3072 (1024 Ge + 2048 Se)

Lattice constant: 46.0x46.0x38.5

The number density: 3072/(46.0x46.0x38.5) = 0.0377 (Å-3) = 3.771022 (cm-3)

**From PRL98**

*“Molecular-dynamics calculations are performed on a system of 648 particles in a cubic cell with periodic boundary conditions. To assess finite-size effects, we have also simulated a system of 5184 particles in a cell whose edge is 55.02 Å in the liquid and 53.75 Å in the glass corresponding to experiment number densities L = 3.114x1022 cm-3 G = 3.338x1022 cm-3, respectively.”*

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For the large systems, the density can be computed by

L = 5184/(55.02x55.02x55.02) = 0.03112 (Å-3)

G = 5184/(53.75x53.75x53.75) = 0.03338 (Å-3)

Since the ratio between the large and small systems is 5184/648 = 8, the lattice constant of the small system are the half 55.02 and 53.75 Å.

**Check on the 2Å peak in gSe-Se(r)**

All QM results (normal density, expansion, contraction) at 1100K have the 2Å peak.

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But QM result at 700K (qm\_700\_GeSe2) does not have the 2Å peak in gSe-Se(r).

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