

MATRL 218: Assignment 4

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1. Use VESTA to sketch the structures of ZnS in the wurtzite and zinc blende structures. Arrange the structures side-by-side so that the ABAB and ABCABC stacking of the two (respectively) become evident. You will need to align the c axis of the wurtzite with a [111] direction of the zinc blende.
2. This is somewhat hard. Can you transform the cubic zinc-blende structure of ZnS so that it can be displayed in a hexagonal cell, with alternating layers of Zn and S along the c axis?
3. Sketch the layered structures of CdI_2 and MoS_2 in VESTA and determine the van der Waals distance between the slabs. This is the perpendicular distance between the anion planes across the gap. VESTA allows planes to be depicted. Try and use these in your solution.
4. Sketch the structure of the cubic perovskite BaZrO_3 with VESTA using the coordinates provided in the notes, indicating ZrO_6 octahedra. Do this with the the given structure, and with the Ba and Zr atoms flipped so that Zr is at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ and Ba is at the origin. Remember to move the O positions appropriately.