HW #3: Interactions - Part I

1. Use *Mathematica* to plot the functional form of de Podesta's Equation 6.6, for a range of A and B values. [The **Manipulate** function can be handy for such exercises.]

2. Given the entries in de Podesta's Table 6.2 for σ and ε for krypton, estimate:
   a) the molar cohesive energy, and
   b) The density

Check your answers by comparing to Table 11.5 and Table 7.2, respectively.

3. Use *Mathematica* to evaluate **Madelung sums** for a 12 x 12 x 12 ionic simple cubic crystal, for an ion near the center. Note that you must take pains to avoid counting the distance from the ion to itself. In particular, to avoid counting the ion at the origin, your sum can be broken into parts. First, you can sum the contributions coming from the 3D region on one side of the plane containing the ion at the origin, and then you can do the same for the 3D region on the other side of the plane containing the ion at the origin. After that, you need to think about the plane containing the ion at the origin. For that plane, first you can sum the contributions coming from the 2D region on one side of the line containing the ion at the origin, and then you can do the same for the 2D region on the other side of the line containing the ion at the origin. Finally, you need to think about the line containing the ion at the origin. For that line, first you can sum the contributions coming from the 1D region on one side of the ion at the origin, and then you can do the same for the 1D region on the other side of the ion at the origin.

— Compare your result to that given for the infinite crystal limit, which is quoted in de Podesta's text on page 155.