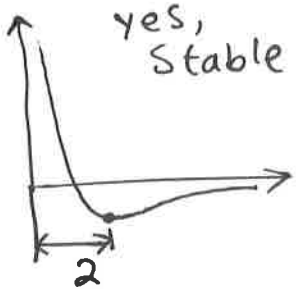
Week 1 - Crystal Binding
Comprehension Check
Total points = 25 (scaled by a factor of 1/10 in the system)

Question 1 (5 points)
The potential energy of a diatomic molecule is given by $U(r) = -1/r + 1/r^2$, with r being the separation distance between the two atoms. Does this configuration lead to a stable bond? If yes, what is the bond length?

$\frac{dU}{dr} = \frac{1}{r^2} - \frac{2}{r^3} = 0 \Rightarrow$ critical point at $r = 2$

$U(2) = -\frac{1}{2} + \frac{1}{4} = -\frac{1}{4}$; $U(\infty) = 0$

$U(0) = \frac{1}{r}\left(-1 + \frac{1}{r}\right) = \frac{1}{0}\left(-1 + \infty\right) \rightarrow \infty$



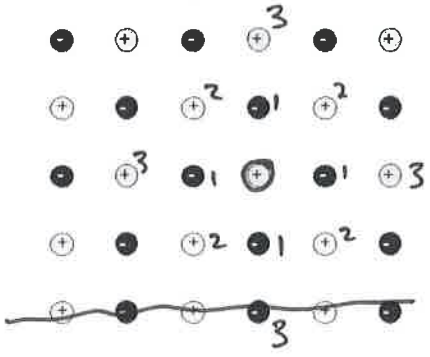
Question 2 (8 points)
Match each of the following bond types to the interaction mechanism involved in the bonding:

1. van der Waals	C	A. Interaction between free electrons and fixed ions
2. Covalent	D	B. Electrostatic potential between oppositely charged ions
3. Metallic	A	C. Dipole-dipole interaction between neutral atoms
4. Ionic	B	D. Sharing of electronic orbitals

Question 3 (6 points)
The ionization energy for atom A is 4 eV. The electron affinity for atom B is 6 eV. The cohesive energy for molecule AB relative to ions A^+ and B^- is 2 eV. Can free atoms A and B join together to form a molecule? Justify your answer.

Loss = 4 eV ionization
Gain = 6ev + 2ev = 8 eV
Gain > Loss => yes, they can join

Question 4 (6 points)



Assume that in this figure the gray and black circles represent oppositely charged ions. Calculate the first <u>three</u> terms in the Madelung's constant.

$\alpha = \frac{4}{1} - \frac{4}{\sqrt{2}} - \frac{4}{2}$

1st 2nd 3rd