PHYSICS OF MATERIALS

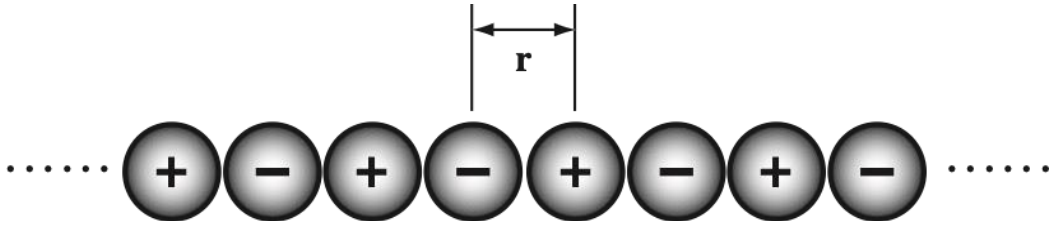
Physics 307 Fall 2024

Series 1 **13 September 2024**

Exercise 1 Madelung constant

Calculate the Madelung s constant for a linear chain of positive and negative ions in the case of a Coulomb potential. Also, try to calculate for a potential with the form:

$$\left(\frac{1}{R^6}\right)$$



Exercise 2 Atomic potential

Van der Waals-type bonds determine the attraction forces of molecules in rare gases. Consider an interaction potential of the type:

$$U = 4\varepsilon\left(\left(\frac{\sigma}{R}\right)^{12} - \left(\frac{\sigma}{R}\right)^{6}\right)$$

Calculate the ratio $\frac{R}{\sigma}$ for two isolated atoms in the FCC structure. Considering that gases interacting with a Van der Waals potential have a compact cubic structure, calculate the equilibrium distance and the cohesion energy following this table:

	Neon	Argon	Krypton	Xenon
σ [Å]	2.8	3.45	3.6	4.06
ε [meV]	2.9	10	14	19

Compare the cohesion energy with those of the table attached and with an ionic compound type such as NaCl (see Chapter I p. 9). Also, compare values of the atomic radii.

Exercise 3 Materials bonding

a) Briefly (3-4 sentences) state ionic, covalent, and metallic bonding differences.

b) State the Pauli exclusion principle as it pertains to atomic bonding theory.

c) Explain why covalently bonded materials are generally less dense than ionically and metallically bonded ones.

Table of Atomic cohesion energies

Li	Be											B	C	N	O	F	Ne
158.	320.											556.	711.	474.	251.	81.0	1.92
1.63	3.32											5.77	7.37	4.92	2.60	0.84	0.020
37.7	76.5											133.	170.	113.4	60.03	19.37	0.46
Na	Mg											Al	Si	P	S	Cl	Ar
107.	145.	← kJ/mol →										327.	446.	331.	275.	135.	7.74
1.113	1.51	← eV/atom →										3.39	4.63	3.43	2.85	1.40	0.080
25.67	34.7	← kcal/mol →										78.1	106.7	79.16	65.75	32.2	1.85
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
90.1	178.	37.6	468.	512.	395.	282.	413.	424.	428.	336.	130.	271.	372.	285.3	217.	118.	11.2
0.934	1.84	3.90	4.85	5.31	4.10	2.92	4.28	4.39	4.44	3.49	1.35	2.81	3.85	2.96	2.25	1.22	0.116
21.54	42.5	89.9	111.8	122.4	94.5	67.4	98.7	101.3	102.4	80.4	31.07	64.8	88.8	68.2	51.8	28.18	2.68
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
82.2	166.	422.	603.	730.	658.	661.	650.	554.	376.	284.	112.	243.	303.	265.	215.	107.	15.9
0.852	1.72	4.37	6.25	7.57	6.82	6.85	6.74	5.75	3.89	2.95	1.16	2.52	3.14	2.75	2.23	1.11	0.16
19.64	39.7	100.8	144.2	174.5	173.3	158.	155.4	132.5	89.8	68.0	26.73	58.1	72.4	63.4	51.4	25.62	3.80
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
77.6	183.	431.	621.	782.	859.	775.	788.	670.	564.	368.	65.	182.	196.	210.	144.		19.5
0.804	1.90	4.47	6.44	8.10	8.90	8.03	8.17	6.94	5.84	3.81	0.67	1.88	2.03	2.18	1.50		0.202
18.54	43.7	103.1	148.4	186.9	205.2	185.2	188.4	160.1	134.7	87.96	15.5	43.4	46.78	50.2	34.5		4.66
Fr	Ra	Ac															
	160.	410.															
	1.66	4.25															
	38.2	98.															

Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
417.	357.	328.		206.	179.	400.	391.	294.	302.	317.	233.	154.	428.
4.32	3.70	3.40		2.14	1.86	4.14	4.05	3.04	3.14	3.29	2.42	1.60	4.43
99.7	85.3	78.5		49.3	42.8	95.5	93.4	70.2	72.3	75.8	55.8	37.1	102.2
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr
598.		536.		347.	264.	372.							
6.20		5.55		3.60	2.73	3.86							
142.9		128.		83.0	63.	89.							

Table of Atomic and ionic radii

H 2,08																	He
Li 0,68 1,56	Be 0,35 1,06 1,13											B 0,23 0,88 0,98	C 0,15 0,77 0,92	N 1,71 0,70	O 1,40 0,66	F 1,36 0,64	Ne 1,58
Na 0,97 1,91	Mg 0,65 1,40 1,60											Al 0,50 1,26 1,43	Si 0,41 1,17 1,32	P 2,12 1,10	S 1,84 1,04	Cl 1,81 0,99	Ar 1,88
K 1,33 2,38	Ca 0,99 1,98	Sc 0,81 1,64	Ti 0,68 1,46	V 1,35	Cr 1,28	Mn 1,26	Fe 1,27	Co 1,25	Ni 1,25	Cu 1,35 1,28	Zn 0,74 1,31 1,39	Ga 0,62 1,26 1,41	Ge 0,53 1,22 1,37	As 2,22 1,18 1,39	Se 1,98 1,14	Br 1,95 1,11	Kr 2,00
Rb 1,48 2,55	Sr 1,13 2,15	Y 0,93 1,80	Zr 0,80 1,60	Nb 0,67 1,47	Mo 1,40	Tc 1,36	Ru 1,34	Rh 1,35	Pd 1,38	Ag 1,26 1,52 1,45	Cd 0,97 1,48 1,57	In 0,81 1,44 1,66	Sn 0,71 1,40 1,55	Sb 2,45 1,36 1,59	Te 2,21 1,32	I 2,16 1,28	Xe 2,17
Cs 1,67 2,73	Ba 1,35 2,24	La 1,15 1,88	Hf 1,58	Ta 1,47	W 1,41	Re 1,38	Os 1,35	Ir 1,36	Pt 1,39	Au 1,37 1,44	Hg 1,10 1,48 1,57	Tl 0,95 1,72	Pb 0,84 1,75	Bi 1,70	Po 1,76	At	Rn
Fr 1,75	Ra 1,37	Ac 1,11															

Ce 1,01 1,71– 1,82	Pr 1,83	Nd 1,82	Pm 1,81	Sm 1,80	Eu $2,04^{2+}$– $1,80^{3+}$	Gd 1,80	Tb 1,78	Dy 1,77	Ho 1,77	Er 1,76	Tm 1,75	Yb $1,94^{2+}$– $1,74^{3+}$	Lu
Th 0,99 1,80	Pa 0,90 1,63	U 0,83 1,56	Np 1,56	Pu 1,58– 1,64	Am 1,81	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Symbole – Mg
0,65 – Radii in layer gas neutrals
1,40 – Radii tetrahedral coordinated covalent bonding
1,60 – Radii for ions in metals with coordination N=12