

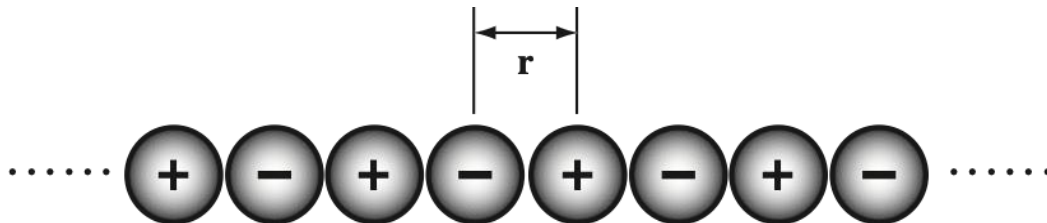
Series 1

12 September 2025

Exercise 1: Madelung constant

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

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

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

Exercise 3 Materials bonding

- Briefly state ionic, covalent, and metallic bonding differences.
- State the Pauli exclusion principle as it pertains to atomic bonding theory.
- Explain why covalently bonded materials are generally less dense than ionically and metallically bonded ones.

Table of Atomic cohesion energies																			
Li 158. 1.63 37.7	Be 320. 3.32 76.5													B 556. 5.77 133.	C 711. 7.37 170.	N 474. 4.92 113.4	O 251. 2.60 60.03	F 81.0 0.84 19.37	Ne 1.92 0.020 0.46
Na 107. 1.113 25.67	Mg 145. 1.51 34.7													Al 327. 3.39 78.1	Si 446. 4.63 106.7	P 331. 3.43 79.16	S 275. 2.85 65.75	Cl 135. 1.40 32.2	Ar 7.74 0.080 1.85
← kJ/mol → ← eV/atom → ← kcal/mol →																			
K 90.1 0.934 21.54	Ca 178. 1.84 42.5	Sc 37.6 3.90 89.9	Ti 468. 4.85 111.8	V 512. 5.31 122.4	Cr 395. 4.10 94.5	Mn 282. 2.92 67.4	Fe 413. 4.28 98.7	Co 424. 4.39 101.3	Ni 428. 4.44 102.4	Cu 336. 3.49 80.4	Zn 130. 1.35 31.07	Ga 271. 2.81 64.8	Ge 372. 3.85 88.8	As 285.3 2.96 68.2	Se 217. 2.25 51.8	Br 118. 1.22 28.18	Kr 11.2 0.116 2.68		
Rb 82.2 0.852 19.64	Sr 166. 1.72 39.7	Y 422. 4.37 100.8	Zr 603. 6.25 144.2	Nb 730. 7.57 174.5	Mo 658. 6.82 173.3	Tc 661. 6.85 158.	Ru 650. 6.74 155.4	Rh 554. 5.75 132.5	Pd 376. 3.89 89.8	Ag 284. 2.95 68.0	Cd 112. 1.16 26.73	In 243. 2.52 58.1	Sn 303. 3.14 72.4	Sb 265. 2.75 63.4	Te 215. 2.23 51.4	I 107. 1.11 25.62	Xe 15.9 0.16 3.80		
Cs 77.6 0.804 18.54	Ba 183. 1.90 43.7	La 431. 4.47 103.1	Hf 621. 6.44 148.4	Ta 782. 8.10 186.9	W 859. 8.90 205.2	Re 775. 8.03 185.2	Os 788. 8.17 188.4	Ir 670. 6.94 160.1	Pt 564. 5.84 134.7	Au 368. 3.81 87.96	Hg 65. 0.67 15.5	Tl 182. 1.88 43.4	Pb 196. 2.03 46.78	Bi 210. 2.18 50.2	Po 144. 1.50 34.5	At	Rn 19.5 0.202 4.66		
Fr	Ra 160. 1.66 38.2	Ac 410. 4.25 98.																	
			Ce 417. 4.32 99.7	Pr 357. 3.70 85.3	Nd 328. 3.40 78.5	Pm	Sm 206. 2.14 49.3	Eu 179. 1.86 42.8	Gd 400. 4.14 95.5	Tb 391. 4.05 93.4	Dy 294. 3.04 70.2	Ho 302. 3.14 72.3	Er 317. 3.29 75.8	Tm 233. 2.42 55.8	Yb 154. 1.60 37.1	Lu 428. 4.43 102.2			
			Th 598. 6.20 142.9	Pa	U 536. 5.55 128.	Np	Pu 347. 3.60 83.0	Am 264. 2.73 63.	Cm 372. 3.86 89.	Bk	Cf	Es	Fm	Md	No	Lr			

Table of Atomic and ionic radii

H 2,08	Table of Atomic and ionic radii																He																																										
Li 0,68	Be 0,35 1,06											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 1,28	Zn 0,74 1,35 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	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	<table border="1"> <tbody> <tr> <td>Ce 1,01 1,71-</td> <td>Pr</td> <td>Nd</td> <td>Pm</td> <td>Sm</td> <td>Eu 2,04²⁺-</td> <td>Gd</td> <td>Tb</td> <td>Dy</td> <td>Ho</td> <td>Er</td> <td>Tm</td> <td>Yb 1,94²⁺-</td> <td>Lu</td> </tr> <tr> <td>1,82</td> <td>1,83</td> <td>1,82</td> <td>1,81</td> <td>1,80</td> <td>1,80³⁺</td> <td>1,80</td> <td>1,78</td> <td>1,77</td> <td>1,77</td> <td>1,76</td> <td>1,75</td> <td>1,74³⁺</td> <td></td> </tr> <tr> <td>Th 0,99 1,80</td> <td>Pa 0,90</td> <td>U 0,83</td> <td>Np</td> <td>Pu 1,58-</td> <td>Am 1,84</td> <td>Cm 1,81</td> <td>Bk</td> <td>Cf</td> <td>Es</td> <td>Fm</td> <td>Md</td> <td>No</td> <td>Lr</td> </tr> </tbody> </table>															Ce 1,01 1,71-	Pr	Nd	Pm	Sm	Eu 2,04 ²⁺ -	Gd	Tb	Dy	Ho	Er	Tm	Yb 1,94 ²⁺ -	Lu	1,82	1,83	1,82	1,81	1,80	1,80 ³⁺	1,80	1,78	1,77	1,77	1,76	1,75	1,74 ³⁺		Th 0,99 1,80	Pa 0,90	U 0,83	Np	Pu 1,58-	Am 1,84	Cm 1,81	Bk	Cf	Es	Fm	Md	No	Lr
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