P#5: Kemijske veze i kohezivna energija

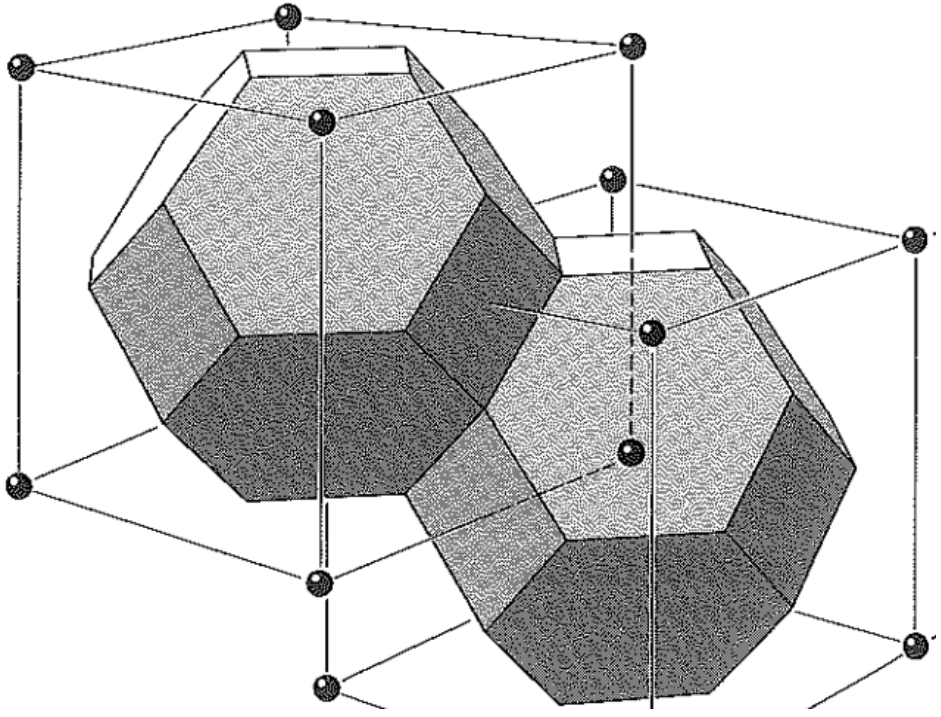
Fizika čvrstog stanja 1

predavanja 2021

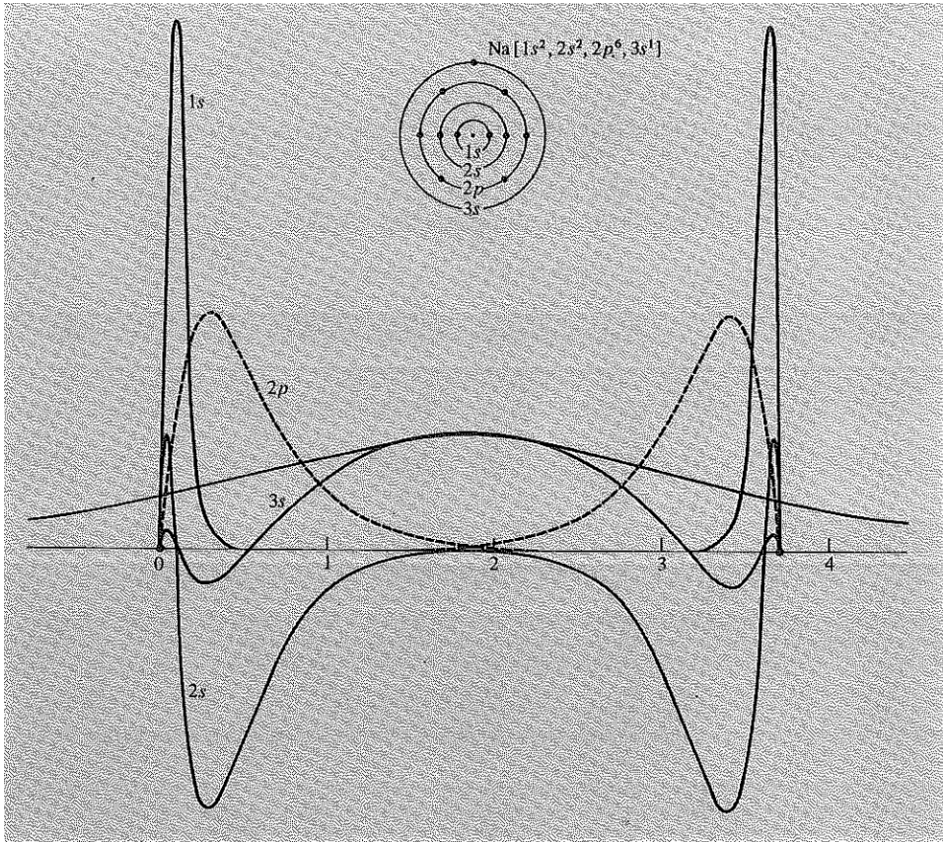
5.1 Kohezivna energija: elementi trećeg retka periodnog sustava

	el. konfig.	E_c (eV/at)	rešetka (prostorna grupa)	vrsta veze
Na	$3s$	1.11	BCC (229)	metalna
Mg	$3s^2$	1.51	HCP (194)	metalna
Al	$3s^2\ 3p$	3.39	FCC (225)	metalna
Si	$3s^2\ 3p^2$	4.63	Dijamant (227)	kovalentna
P	$3s^2\ 3p^3$	3.43	Triklinska (2)	kovalentna
S	$3s^2\ 3p^4$	2.85	FC Ortorombska (70)	kovalentna
Cl	$3s^2\ 3p^5$	1.40	BC Ortorombska (64)	kovalentna
Ar	$3s^2\ 3p^6$	0.08	FCC (225)	Van der Waalsova

5.2 Wigner-Seitzov račun kohezivne energije: alkalijski metali, BCC Bravaisova rešetka



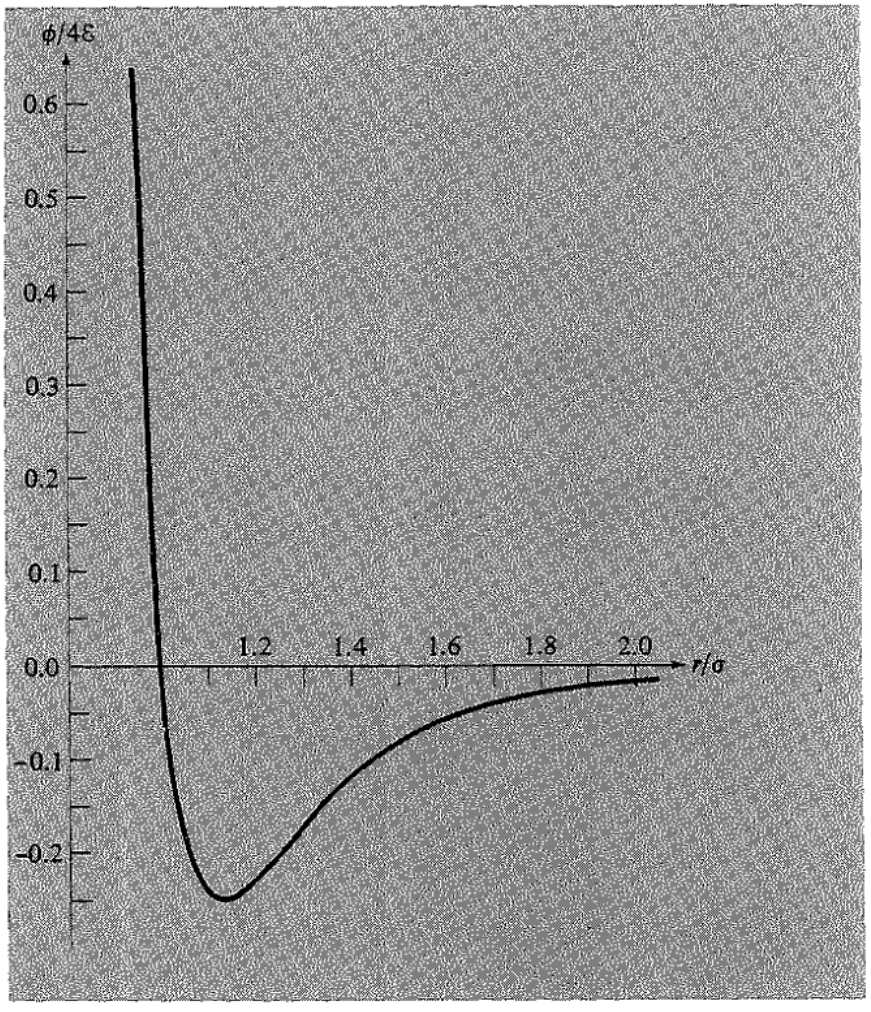
izračunate valne funkcije elektrona $u_{nl}(r)$ u atomskom natriju



5.3 Kohezija kristala plemenitih plinova

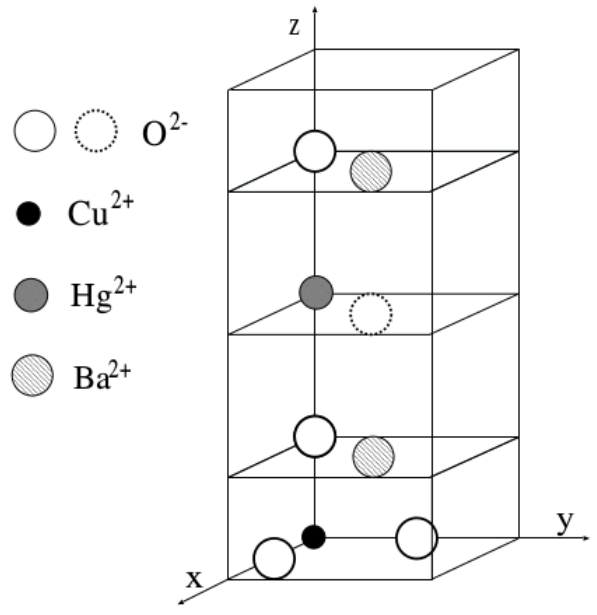
	rešetka	d_{at-at} (Å)	E_c (eV/at)	Talište (K)
Ne	FCC	3.13	0.020	24
Ar	FCC	3.76	0.080	84
Kr	FCC	4.01	0.116	117
Xe	FCC	4.35	0.17	161

6-12 Lennard-Jonesov potencijal

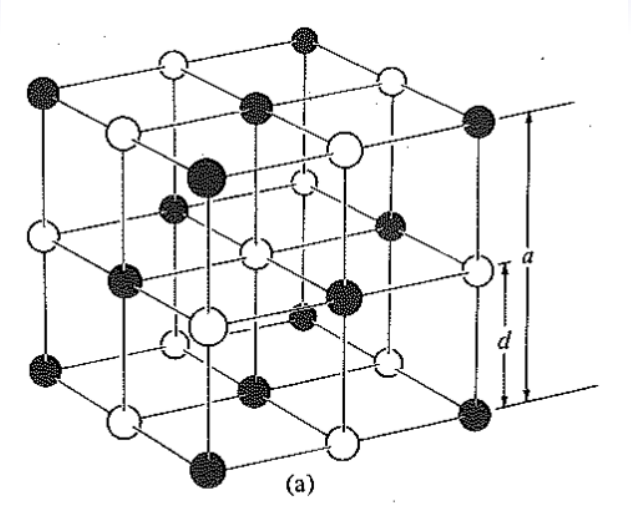


teorijska predviđanja za kristale plemenitih plinova

		Ne	Ar	Kr	Xe
r_0 (angstroms)	(Experiment)	3.13	3.75	3.99	4.33
$r_0 = 1.09\sigma$	(Theory)	2.99	3.71	3.98	4.34
u_0 (eV/atom)	(Experiment)	−0.02	−0.08	−0.11	−0.17
$u_0 = -8.6\epsilon$	(Theory)	−0.027	−0.089	−0.120	−0.172
B_0 (10^{10} dyne/cm^2)[b]	(Experiment)	1.1	2.7	3.5	3.6
$B_0 = 75\epsilon/\sigma^3$	(Theory)	1.81	3.18	3.46	3.81



Slika 1.2: Atomi u primitivnoj ćeliji (ili bazi) supravodiča $HgBa_2CuO_{4+\delta}$. Kristal se sastoji od izolatorskih HgO_δ i BaO ravnina i (supra)vodljivih CuO_2 ravnina.

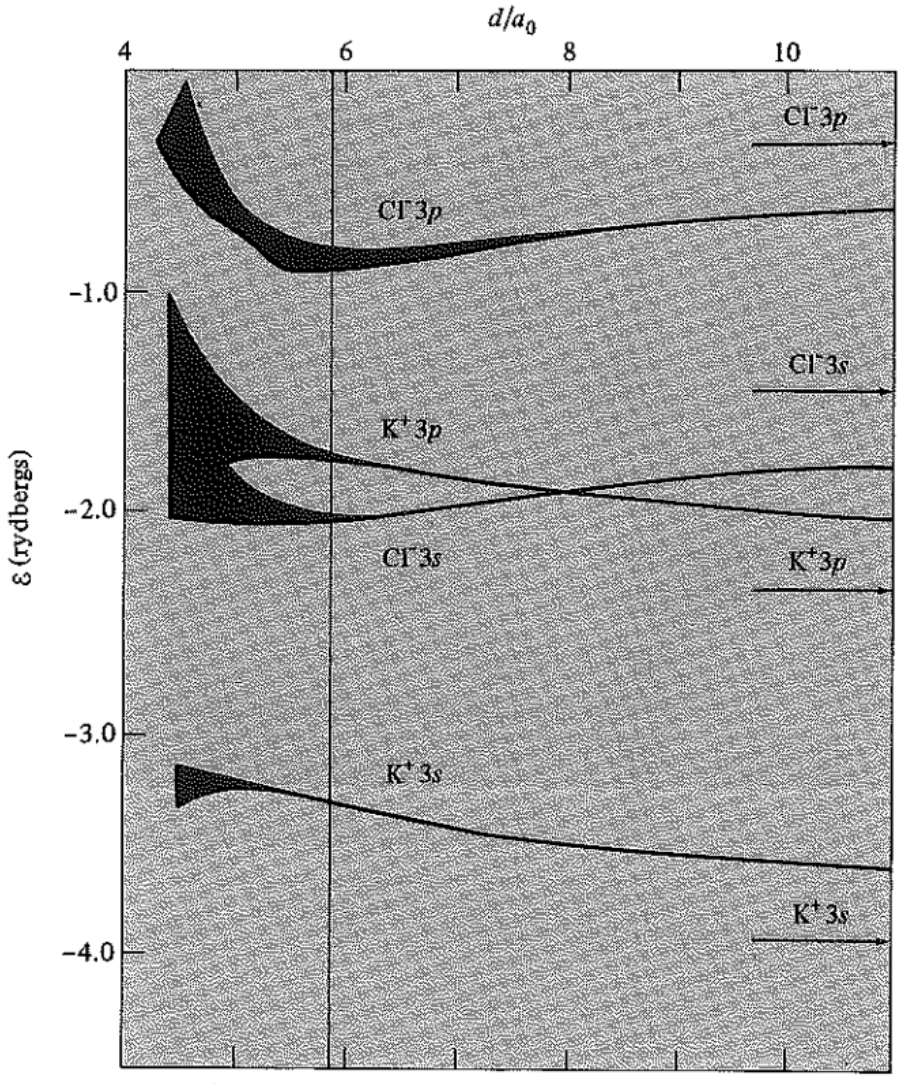


(a)

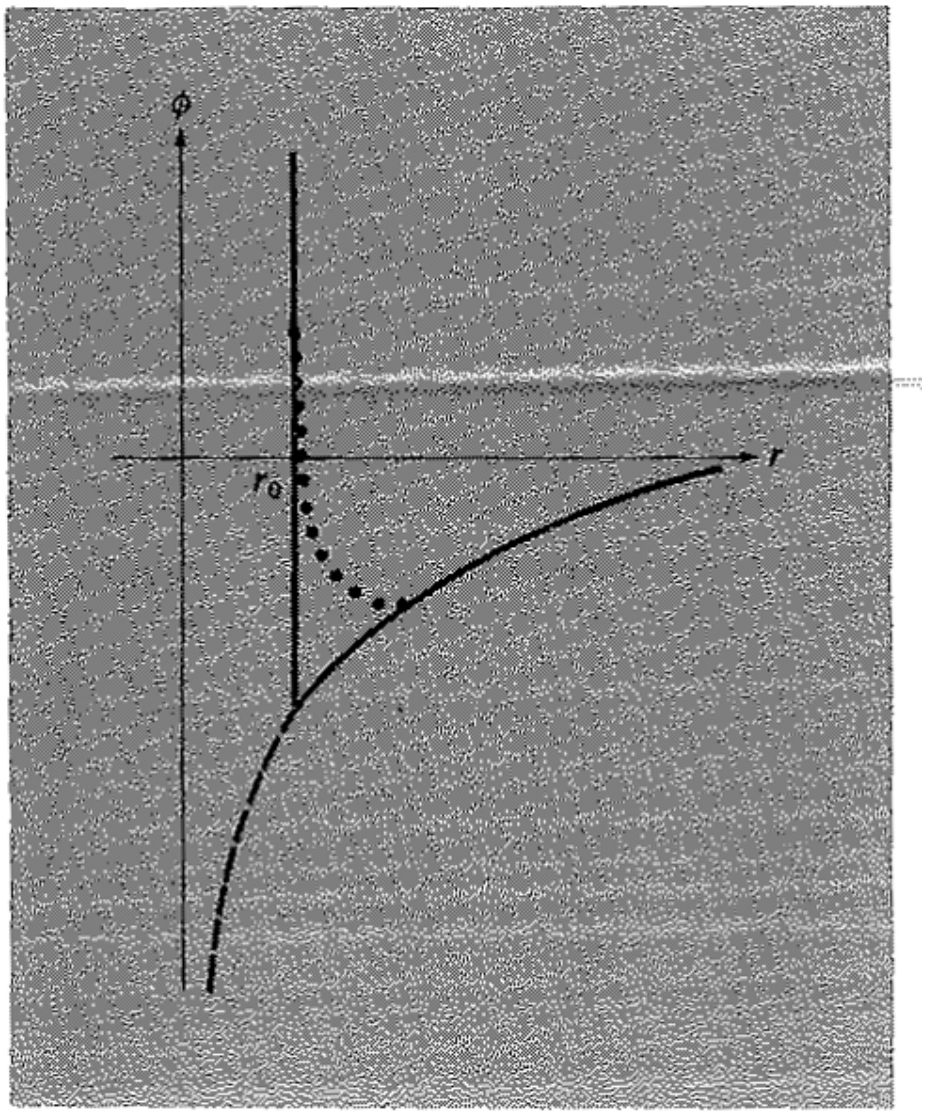
SOME COMPOUNDS WITH THE SODIUM CHLORIDE STRUCTURE

CRYSTAL	a (Å)	CRYSTAL	a (Å)	CRYSTAL	a (Å)
LiF	4.02	RbF	5.64	CaS	5.69
LiCl	5.13	RbCl	6.58	CaSe	5.91
LiBr	5.50	RbBr	6.85	CaTe	6.34
LiI	6.00	RbI	7.34	SrO	5.16
NaF	4.62	CsF	6.01	SrS	6.02
NaCl	5.64	AgF	4.92	SrSe	6.23

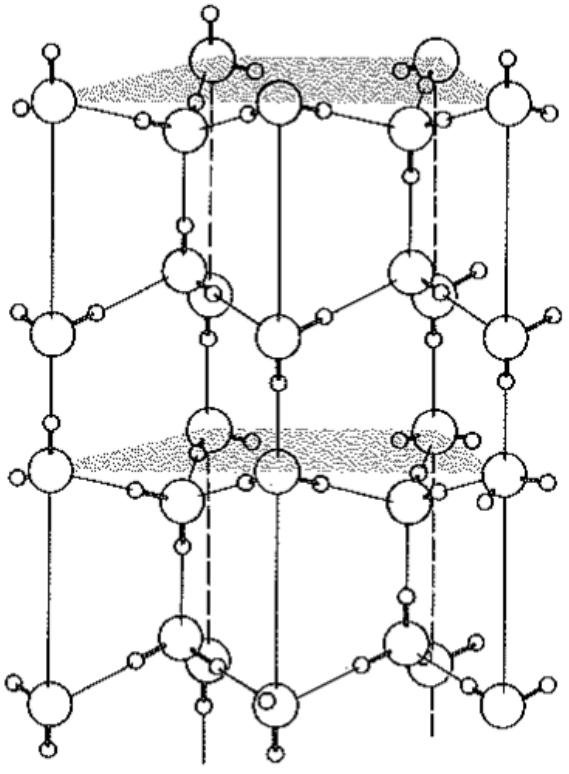
širina valentnih vrpci u ionskom kristalu KCl



kohezivna energija



5.6. Vodikova veza



Literatura

1) Ashcroft & Mermin, *Solid State Physics*, §§ 19.2, 19.3, 19.6, 19.8, 20.U - 20.2
2) Anderson, *Concepts in Solids*, § 2.B.2
3) Kittel, *Introduction to Solid State Physics*, §§ 3.U - 3.2
4) bilješke