PHYS 321 F 2019 Test #1 Name: Key

A. Uranium metal can be produced by the reaction of uranium tetrafluoride (UF_4) with magnesium (Mg) in a sealed reactor heated to 700°C. The by-product is magnesium fluoride (MgF_2). To ensure that all the magnesium is consumed in the reaction, the reactor is charged with excess UF_4, specifically 12% more than the stoichiometric requirement of the reaction. To produce 322 kg of U, how much UF_4 and Mg must be introduced into the reactor? Express your answers in kg. (U:238, F:19.0, Mg:24.3)

$UF_4 + 2Mg \longrightarrow U + 2MgF_2$

$UF_4 = 314$

$\frac{322 \times 10^3}{238} = 1353$ mol of U

UF_4: $1.12 \times \frac{1353 \times 314}{1000}$ kg $= 476$ kg

\# of mol of Mg $= 2 \times 1353 = 2706$

Mg: $2706 \times 24.3/1000 = 66$ kg

28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.38
46 Pd Palladium 106.42	47 Ag Silver 107.87	48 Cd Cadmium 112.41

B. Give the electron configurations for: Cu and Cu^+

Cu: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$

Cu^+: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10}$

C1. Compute the percent ionic character of the inter-atomic bonds for the following compound: CdTe. 3.92%

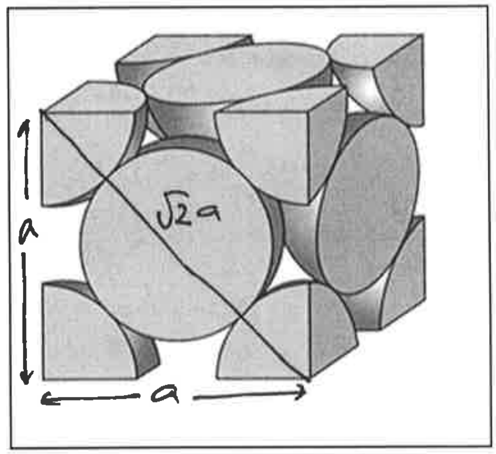
C2. On the basis of the above result what type of interatomic bonding would you expect in CdTe? Covalent

The electronegativity values are given below.

$$\%\text{ ionic character} = \left(1 - e^{-\frac{(X_A - X_B)^2}{4}}\right) \times (100\%)$$

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII	VIII	VIII	IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
1 H 2.1																	2 He -
3 Li 1.0	4 Be 1.5											5 B 2.0	6 C 2.5	7 N 3.0	8 O 3.5	9 F 4.0	10 Ne -
11 Na 0.9	12 Mg 1.2											13 Al 1.5	14 Si 1.8	15 P 2.1	16 S 2.5	17 Cl 3.0	18 Ar -
19 K 0.8	20 Ca 1.0	21 Sc 1.3	22 Ti 1.5	23 V 1.6	24 Cr 1.6	25 Mn 1.5	26 Fe 1.8	27 Co 1.8	28 Ni 1.8	29 Cu 1.9	30 Zn 1.6	31 Ga 1.6	32 Ge 1.8	33 As 2.0	34 Se 2.4	35 Br 2.8	36 Kr -
37 Rb 0.8	38 Sr 1.0	39 Y 1.2	40 Zr 1.4	41 Nb 1.6	42 Mo 1.8	43 Tc 1.9	44 Ru 2.2	45 Rh 2.2	46 Pd 2.2	47 Ag 1.9	48 Cd 1.7	49 In 1.7	50 Sn 1.8	51 Sb 1.9	52 Te 2.1	53 I 2.5	54 Xe -
55 Cs 0.7	56 Ba 0.9	57-71 La-Lu 1.1-1.2	72 Hf 1.3	73 Ta 1.5	74 W 1.7	75 Re 1.9	76 Os 2.2	77 Ir 2.2	78 Pt 2.2	79 Au 2.4	80 Hg 1.9	81 Tl 1.8	82 Pb 1.8	83 Bi 1.9	84 Po 2.0	85 At 2.2	86 Rn -
87 Fr 0.7	88 Ra 0.9	89-102 Ac-No 1.1-1.7															

D. The unit cell for the face-centered cubic crystal structure is shown below.



1. Show that the cube edge length, a and the atomic radius, R are related by: $a = 2R\sqrt{2}$

$a^2 + a^2 = (4R)^2$

$2a^2 = 16R^2$

$a = \sqrt{8} \cdot R = \sqrt{8}\,R$

$a = 2\sqrt{2}\,R$

2. Show that the atomic packing factor is 0.74 for FCC.

$$APF = \frac{\text{Vol. of atom}}{\text{vol. of cube}} = \frac{\frac{4}{3}\pi R^3 \times 4}{a^3}$$

$$= \frac{\frac{4}{3}\pi R^3 \times 4}{(2\sqrt{2}R)^3} = \frac{\frac{16}{3}\pi}{(2\sqrt{2})^3} = \underline{0.74}$$

3a. Calculate the atomic radius of a copper atom, given that Cu has a FCC crystal structure, a density of 8.94 g/cm^3, and an atomic weight of 63.546 g/mol.

$$\rho = \frac{m}{V} \rightarrow V = \frac{m}{\rho} = \frac{4 \times 63.546}{6.022 \times 10^{23} \times 8.94} = a^3 = 4.72 \times 10^{-23}\ cm^3$$

$$a = \left(\frac{4 \times 63.546}{6.022 \times 10^{23} \times 8.94}\right)^{1/3} = 3.61 \times 10^{-8}\ cm$$

$$a = 2\sqrt{2}R \rightarrow R = \frac{a}{2\sqrt{2}} = \frac{3.61 \times 10^{-8}}{2\sqrt{2}} = 1.28 \times 10^{-8}\ cm = 0.128 \times 10^{-7}\ cm$$

$R = 0.128\ nm$

3b. Calculate the linear density for [111] direction and planar density for (111) planes in copper.

$$LD[111] = \frac{1}{\sqrt{3}\,a} = \frac{1}{\sqrt{3} \cdot 2\sqrt{2}R}$$

$$= \frac{1}{2\sqrt{6}\,R}$$

$$= \frac{1}{2\sqrt{6} \times 0.128\ nm}$$

$LD[111] = 1.595\ nm^{-1}$

$LD[111] = 1.595 \times 10^{7}\ cm^{-1}$

$h = 4R \sin 60^\circ$

$h = 2\sqrt{3}R$

$A = \frac{1}{2} \times 4R \times 2\sqrt{3}R$

$A = 4\sqrt{3}R^2$

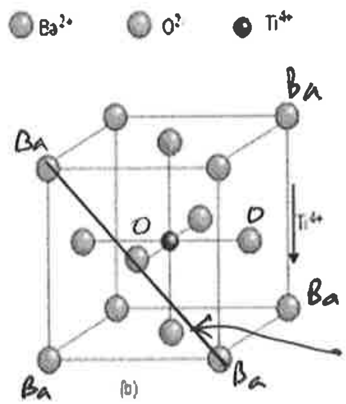
$$PD_{(111)} = \frac{2}{4\sqrt{3}R^2} = \frac{1}{2\sqrt{3}R^2}$$

$$= \frac{1}{2\sqrt{3} \times 0.128^2}\ nm^{-2} = 17.6\ nm^{-2}$$

$= 17.6 \times 10^{14}\ cm^{-2}$

$PD_{(111)} = 1.76 \times 10^{15}\ cm^{-2}$

E. Determine the density of $BaTiO_3$, which forms a perovskite crystal structure, shown below:



	Ionic Radius (nm)	Atomic mass (g/mol)
Ba (Corner)	0.136	137.3
O (Face center)	0.140	16
Ti (Middle)	0.145	47.87

atoms are touching along face-diagonal.

$d = 2R_{Ba} + 2R_O = 2\times0.136 + 2\times0.140$

$d = 0.552 nm$

$d^2 = a^2 + a^2 = 2a^2$

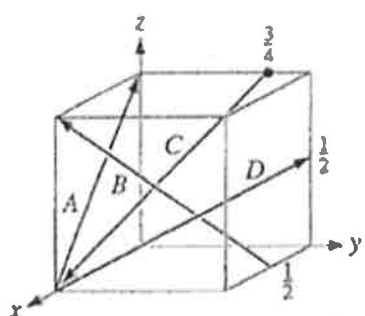
$d = \sqrt{2}a = 0.552$

$a = \frac{0.552}{\sqrt{2}} = 0.3903 nm$

$\rho = \frac{m}{V} = \frac{(47.87 + 137.3 + 3\times16)/6.022\times10^{23}}{(0.3903\times10^{-7})^3 cm^3} = 6.51 \frac{g}{cm^3}$

$\rho_{BaTiO_3} = 6.51 \frac{g}{cm^3}$

F. What are the indices for the directions represented by the vectors (A,B,C,D) that has been drawn within a unit cell?



A: Tip 0 0 1
Tail 1 0 0
-1 0 1
$[\bar{1}01]$

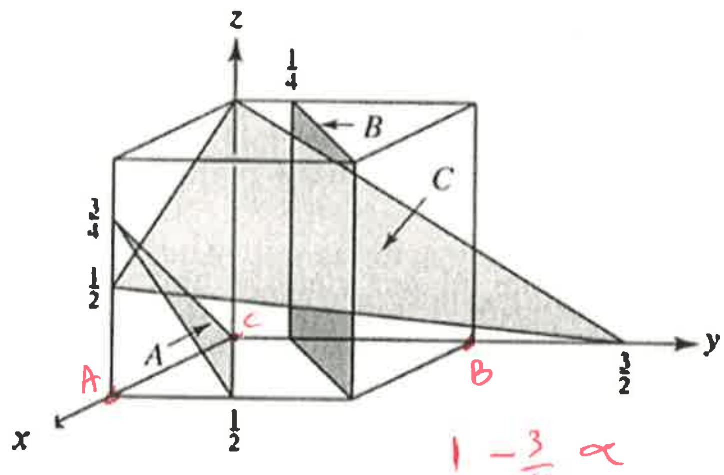
B:
1 0 1
$\frac{1}{2}$ 1 0
$\frac{1}{2}$ -1 1
1 -2 2
$[1\bar{2}2]$

C: 1 0 0
0 $\frac{3}{4}$ 1
1 $-\frac{3}{4}$ -1
4 -3 -4
$(4\bar{3}\bar{4})$

D: 0 1 $\frac{1}{2}$
1 0 0
-1 1 $\frac{1}{2}$
-2 2 1
$[\bar{2}21]$

OR 0 1 $\frac{1}{2}$
0 0 0
0 1 $\frac{1}{2}$
0 2 1
$[021]$

G. Determine the Miller indices for the planes shown (A,B,C) in the following unit cell:



$-1 \quad \frac{1}{2} \quad \frac{3}{4}$

$-1 \quad 2 \quad \frac{4}{3}$

$-3 \quad 6 \quad 4$

$(\bar{3}\,6\,4)$

$1 \quad -\frac{3}{4} \quad \infty$

$1 \quad -\frac{4}{3} \quad 0$

$(3\,\bar{4}\,0)$

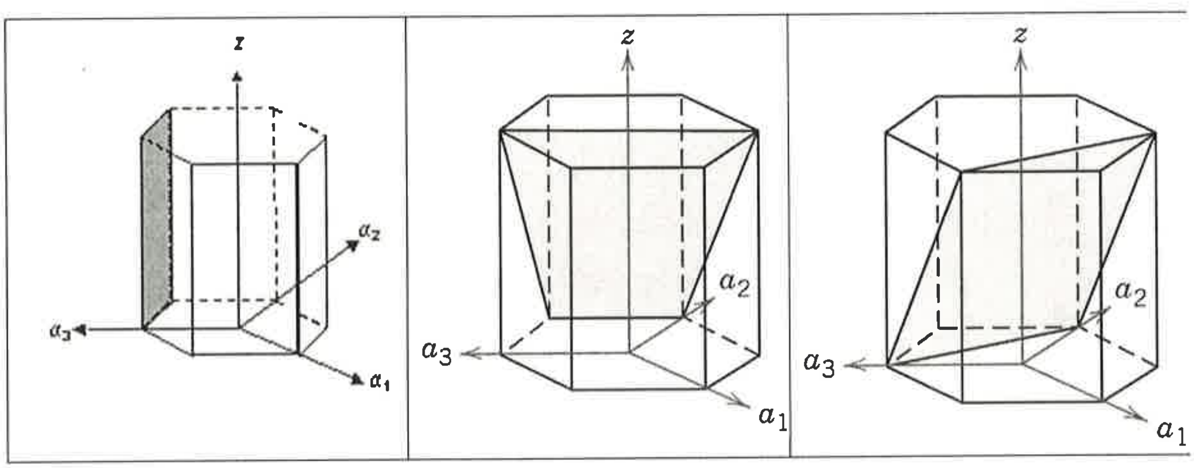
C $2 \quad \frac{3}{2} \quad 1$

$\frac{1}{2} \quad \frac{2}{3} \quad 1$

$6(\frac{1}{2} \; \frac{2}{3} \; 1)$

$(3\,4\,6)$

H. What are the Miller indices for the planes shown below?



$-1 \quad \infty \quad 1 \quad \infty$

$(\bar{1}\,0\,1\,0)$

$-1 \quad 1 \quad \infty \quad 1$

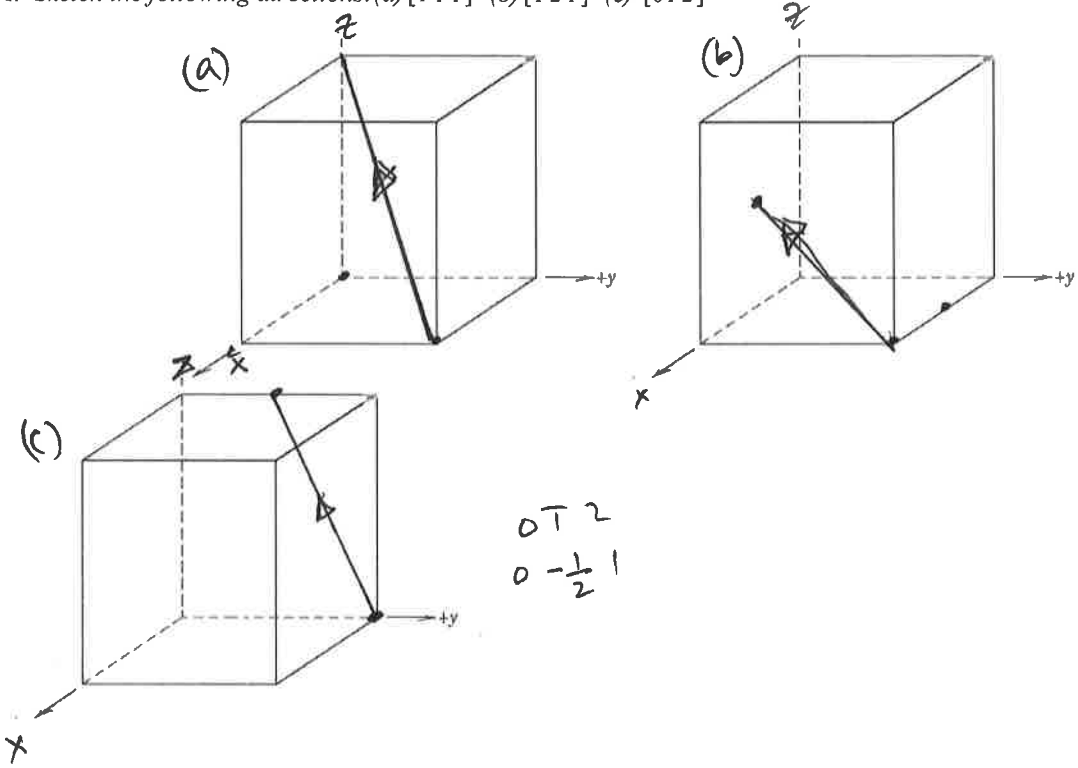
$(\bar{1}\,1\,0\,1)$

$-\frac{1}{2} \quad 1 \quad 1 \quad \frac{1}{2}$

$-2 \quad 1 \quad 1 \quad 2$

$(\bar{2}\,1\,1\,2)$

I. *Sketch the following directions: (a)* $[\bar{1}\bar{1}1]$ *(b)* $[\bar{1}\bar{2}1]$ *(c)* $[0\bar{1}2]$



$\bar{1}\ \bar{2}\ 1$

$-\frac{1}{2}\ -1\ \frac{1}{2}$

$0\ \bar{1}\ 2$

$0\ -\frac{1}{2}\ 1$

J. *Sketch* $[1\bar{2}\bar{2}3]$ *and* $[\bar{2}4\bar{2}3]$ *direction in a hexagonal unit cell.*

$\bar{2}\ 4\ \bar{2}\ 3$

$-\frac{2}{6}\ \frac{4}{6}\ -\frac{2}{6}\ \frac{3}{6}$

$-\frac{1}{3}\ \frac{2}{3}\ -\frac{1}{3}\ \frac{1}{2}$

$\frac{1}{3}\ -\frac{2}{3}\ -\frac{2}{3}\ 1$