Supplemental Problems for Chapter 1

1. The August 2000 issue of the Materials Research Society Bulletin was focused on the topic "Transparent Conductors"; the title refers to materials that are both transparent to light and electronically conductive.

(i) Suitable materials for applications where both properties are needed (for example, in thin film photovoltaics, flat screen displays, and electrochromic windows) are very rare. Explain why you think that this is the case.

(ii) Among the binary phases that can be used as transparent conductors are SnO_2, In_2O_3, and ZnO. How would you classify the bonding in these compounds?

(iii) Ternary phases that can be used as transparent conductors are $ZnSnO_3$, $In_4Sn_3O_{12}$, $GaInO_3$, $Zn_2In_2O_5$. How would you classify the bonding in these compounds?

(iv) What do the transparent conducting phases have in common?

(v) Use radius ratio rules to predict the coordination number of the more metallic element in SnO_2, In_2O_3, and ZnO. Do the predictions compare well with what is known about the structures of these phases?

2. High thermal conductivity materials are those that have a thermal conductivity (κ) greater than 100 W m^{-1} K^{-1}. The table below lists several of these materials.

Crystal	**κ, (W m^{-1} K^{-1})**
Graphite	2000
Diamond	2000
BN	1300
SiC	490
BeO	370
BP	360
AlN	320
BeS	300
BAs	210
GaN	170
Si	160
AlP	130
GaP	100

(i) How would you characterize the bonding in these materials?
(ii) What types of structures are these compounds most likely to adopt?
(iii) Can you identify any periodic trends in the thermal conductivity? Consider, for example, mass, mass difference, electronegativity, and electronegativity difference.

3) The table below lists the melting points (T_m) of several carbide phases. These "hard metals" are used in applications such as cutting and machining where high wear resistance, hardness, and toughness are all required.

Phase	T_m °C	Phase	T_m °C
TiC	3100	NbC	3600
ZrC	3400	TaC	3800
HfC	3900	MoC	2500
VC	2700	WC	2800

(i) How would you describe the bonding in these materials? (metallic, ionic, or covalent) Justify your choice.
(ii) All of the metal atoms in these compounds are approximately twice the radius of C. How do you think that C is coordinated in these crystal structures? Explain the reason for your choice.
(iii) Based on the stoichiometry and coordination, which of the prototype structures do you think these phases might adopt?
(iv) Is there a correlation between the fractional ionicity of bonding in these compounds and their melting points?