

## Survey of Materials

### Homework 1 – Solution

1. (A), maximal voltage mainly depends on ion intercalation energy, which in turn is defined by atomistic structure of electrode material.
2. (C,F,G)
3. (B,C,D,F)
4. (E)
5. Covalently bound dimers with metallic bonding between them.
6. CC, CCC,  $2\times\text{CH}$ , HCH;  $T_d=-43m$ , HC-CH.
7.  $a, c$ ; P63/mmc; C-C.
8. See TiO2\_anatase\_labels.cif. Space group is I41/amd:1. Voids are at  $(4b)=(0,0,1/2)$ , bonds are at  $(8e)=(0,0,\xi)$ ,  $0 < \xi < \xi_O$  and  $(16h)=(0,\eta,\zeta)$ . Miller indexes are  $\{102\}$ .
9. Band gap is 1 eV (indirect) and 2.5 eV for direct. Bandwidth for holes is 5 eV, for electrons is  $\geq 5$  eV. Covalent crystal of elements of main groups 2-6 with average valence close to 4, rows Si to Sn.