

Survey of Materials

Homework 3 – Solution

1. The electrode potential in addition to ionization and cohesive energies depends on hydration enthalpy of cation. Being the smallest cation, Li^+ forms the strongest bonds with oxygen, and as a result has the most negative hydration enthalpy (-5.4 eV).

2. The specific capacity (C) is amount of stored charge per unit of mass of material. For given chemical formula, $C = eN_A/M$, where e is electron charge ($1.6 \times 10^{-19} \text{ C}$), N_A is Avogadro constant (6.02×10^{23}) and M is molar weight of compound.

$C(\text{LiCoO}_2) = 273 \text{ mAh/g}$, $C(\text{Li}_2\text{CoPO}_4\text{F}) = 286 \text{ mAh/g}$, $C(\text{Na}_2\text{CoPO}_4\text{F}) = 244 \text{ mAh/g}$.

3. The catalytic activity of perovskites ABO_3 (B is transition metal) in oxygen reduction reaction (ORR) implies B-OH^- breaking and formation of B-O_2^{2-} and then back B-OH^- regeneration, which are considered rate limited processes. The antibonding electron at e_g orbital promotes the formation of B-O_2^{2-} bonds instead of B-OH^- . However, more than one antibonding electron starts to destabilize B-O_2^{2-} . Less than one electron results in too stable B-O_2^{2-} , preventing B-OH^- regeneration. As a result, “volcano plot” of catalytic activity is observed with maximum at single electron filling.

4. (A,B,D,F). Electron injection effectiveness depends on LUMO level of an organic semiconductor relative to the electrode work function.

5. (C), also (B)

6. Proper functionalization of a CNT according to the given matrix material: COOH , alkyl chains. Hydrogen termination of CNT ends.