

Supporting Information

Estimation of electrochemical cell potentials and reaction energies using Fermi energies

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Methodology Details

Inside the non-overlapping spheres of muffin tin radius (R_{MT}) around each atom, linear combination of radial solution of the Schrödinger equation times the spherical harmonic are used and the plane wave basis set is used in the interstitial region. To expand the wave functions in the interstitial region a plane wave cut-off value of $K_{max} \cdot R_{mt} = 7.0$ was used, where R_{mt} is the smallest atomic sphere radius in the unit cell and K_{max} is the magnitude of the largest K vector. The Fourier-expanded charge density was truncated at $G_{max} = 12$ (Ryd)^{1/2}. The maximum value of the angular momentum (l_{max}) was set equal to 10 for the wave function expansion inside the atomic spheres.

Spheres of muffin tin radius (R_{MT}) around each atom were dictated by structure for each material. In the case of Li_2FeSiO_4 , $LiFePO_4$, $LiCoO_2$, $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$ (NCM), and $LiMn_2O_4$, R_{MT} values 1.76, 2.00, 2.00 and 2.02 a.u. were used for Li, Mn, Fe and Co, respectively, and 1.42 a.u. for Si, P and O atoms. For $LiFeBO_3$, R_{MT} of Fe, Li, B and O atoms set at 2.00, 1.75, 1.28 and 1.28 a.u., respectively. In the case of $LiFeSO_4F$, R_{MT} of Fe, Li, S, F and O atoms was equal to 1.96, 1.82, 1.35, 1.74 and 1.35 a.u., respectively. The electron and spin configuration of the atoms were software defaults and were: Li: [He] 2s¹, B: [He] 2s² 2p¹, O: [He] 2s² 2p⁴, F: [He] 2s² 2p⁵, Si: [Ne] 3s² 3p², P: [Ne] 3s² 3p³, S: [Ne] 3s² 3p⁴, Mn_{up} : [Ar] 3d⁵(5↑, 0↓) 4s²(1↑, 1↓), Fe_{up} : [Ar] 3d^{6.5}(4.5↑, 2↓) 4s^{1.5}(1↑, 0.5↓) and Co_{up} : [Ar] 3d⁷(5↑, 2↓) 4s²(1↑, 1↓).