Simple LCAO model

N. A. W. Holzwarth[†]

Department of Physics, Wake Forest University, Winston-Salem, NC 27109

Abstract

[†]natalie@wfu.eduYour e-mail address; http:
www.wfu.eduñatalieYour web page

I BASIC EQUATIONS

The purpose of this formalism is to provide a simple and reasonable interpolation scheme to model ionic materials.

The model has the following components:

1. Each ion has a position index $\mathbf{R}$ and a positive charge $Q_{\mathbf{R}}$. The charge $Q_{\mathbf{R}} \equiv Z_{\mathbf{R}} - z_{\mathbf{R}}^{core}$ includes the nuclear charge $Z_{\mathbf{R}}$ and the core electron $z_{\mathbf{R}}^{core}$ contributions. In the model, it is represented by a spherical charge density shape function $S_{\mathbf{R}}(r)$ (assumed to be normalized to unity such as a Gaussian form $S_{\mathbf{R}}(r) = e^{-(r/\sigma_{\mathbf{R}})^2}/(\pi^{3/2}\sigma^3)$) so the total density associated with the ions of the material is represented by

$$\rho^{ion}(\mathbf{r}) = \sum_{\mathbf{R}} Q_{\mathbf{R}} S_{\mathbf{R}}(|\mathbf{r} - \mathbf{R}|). \tag{1}$$

2. In addition to its charge distribution, each ion has an associated spherically symmetric local potential which is used to adjust the model electron affinities and negativities described by an amplitude $\mathcal{V}_{\mathbf{R}}$ and shape function $\Phi_{\mathbf{R}}(r)$ so that the total local potential of the material is given by

$$V^{loc}(\mathbf{r}) = \sum_{\mathbf{R}} \mathcal{V}_{\mathbf{R}} \Phi_{\mathbf{R}}(|\mathbf{r} - \mathbf{R}|). \tag{2}$$