Attempt at explanation of PDOS for Quantum Espresso in PAW mode

The partial densities of states were calculated as programmed in the *Quantum Espresso*[1] package. The evaluation replaces the delta function of the densities with a Gaussian function of width $\sigma = 0.01$ eV. The local density of states weight factor $Q^a_{n\mathbf{k}}$ for atomic site a and of band index n and wave vector $\mathbf{k}$, is determined by matrix elements of the form $\langle \widetilde{p}^a_i | \widetilde{\Psi}_{n\mathbf{k}} \rangle$. Here $|\widetilde{\Psi}_{n\mathbf{k}}\rangle$ represents the pseudo-wavefunction and $|\widetilde{p}^a_i\rangle$ represents the PAW atomic projector function which is localized within the augmentation sphere about the atomic site a and i denotes radial and spherical harmonic index of the projector function.[2, 3] The explicit form of the partial density of states weight factor for an atom on site a for the state $n\mathbf{k}$ is given by

$$Q^a_{n\mathbf{k}} = \sum_i |\langle \widetilde{p}^a_i | \widetilde{\Psi}_{n\mathbf{k}} \rangle|^2. \tag{1}$$

Because of the PAW formalism, each term in the summation represents the expansion coefficient for the eigenfunction $n\mathbf{k}$ in each augmentation sphere a in the set of atom-centered basis functions i. While the value of $Q^a_{n\mathbf{k}}$ will depend on the choice of basis functions in the PAW dataset, we find the results of this analysis to qualitatively agree with previous work[4, 5] where the charge was directly integrated within the augmentation sphere.

References

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