

Erratum to: A First-Principles Study of the Role of Na Vacancies in the Thermoelectricity of Na_xCoO_2

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An incorrect value for π , 34.1415926535897 9323846 instead of 3.14159265358979323846, was inadvertently used when calculating the change in

charge density upon formation of a sodium vacancy as a function of radial distance from the nuclei of various species, specifically when the change in the charge density was divided by the volume of a spherical shell, $\frac{4}{3} \cdot \pi(r_+^3 - r_-^3)$, where r_+^3 and r_-^3 denote outer and inner radii of the shell, respectively. The values plotted in Fig. 3 and Fig. 4 are

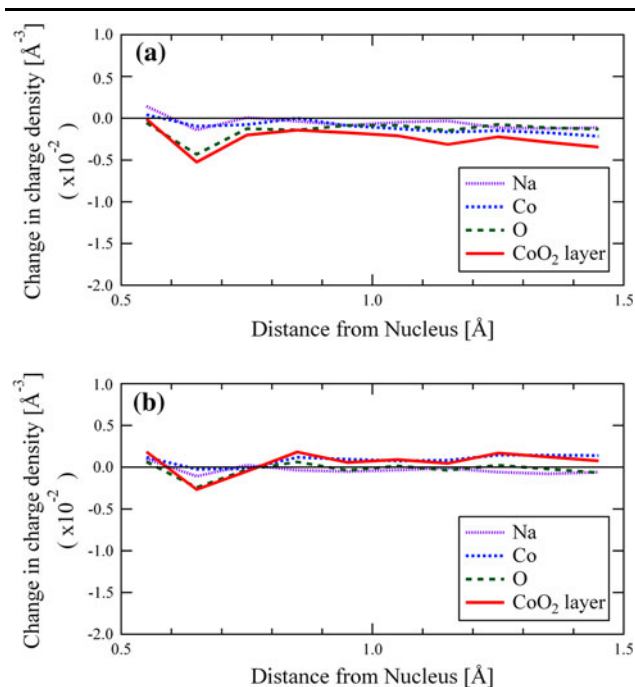


Fig. 3. Charge density distributions per unit volume in 1 \AA thick spherical shells about the nuclei of various species. For CoO_2 units, the sum of the charge density for Co and twice the charge density for O is used. (a) Change upon formation of V_{Na} in NaCoO_2 and (b) change upon formation of V_{Na} in NaCoO_2 . Comparison of the two plots shows the change in electronic structure upon removal of the electron needed to maintain charge neutrality when the Na vacancy is formed.

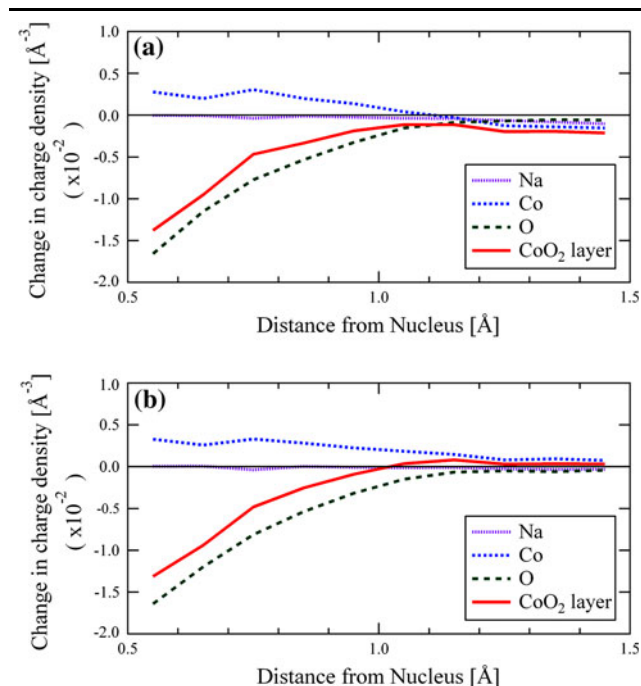


Fig. 4. Charge density distributions per unit volume in spherical shells about the nuclei of various species. For CoO_2 units, the sum of the charge density for Co and twice the charge density for O is plotted. (a) Change upon formation of V_{Na} in $\text{Na}_{0.5}\text{CoO}_2$ and (b) change upon formation of V_{Na} in $\text{Na}_{0.5}\text{CoO}_2$. Comparison of the two plots shows the change in electronic structure upon removal of the electron needed to maintain charge neutrality when the Na vacancy is formed.

thus approximately one order of magnitude smaller than they should be. However, since the discussion and conclusions were based simply on whether the

changes in charge density were positive or negative, these remain unaffected. The corrected figures are shown above.