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Beyond the Rigid-Ion Approximation with Spherically Symmetric Ions

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Beyond the Rigid-Ion Approximation with Spherically Symmetric Ions. L. L. BOYER, M. J. MEHL, J. L. FELDMAN, J. R. HARDY, J. W. FLOCKEN, and C. Y. FONG [Phys. Rev. Lett. **54**, 1940 (1985)].

In our recent Letter we introduced an *ab initio* model for spherically symmetric charge relaxation of ions in a crystal, called potential-induced breathing (PIB), and demonstrated its importance in the calculation of elastic constants. We also investigated the splitting of the longitudinal optic (LO) and transverse optic (TO) mode frequencies, which results from the macroscopic field associated with longitudinal modes. In the discussion immediately before and after Eq. (5) we argued, incorrectly, that the only contributions to the LO-TO splitting from PIB were from terms involving S'_k , the derivative of the self-energy of the k th ion with respect to the electrostatic potential at the k th-ion site. In fact, other terms within the PIB model contribute as well. Further study has shown that the treatment of macroscopic field effects in the PIB model is not straightforward. This will be discussed in a future paper (R. E. Cohen, L. L. Boyer, and M. J. Mehl, to be published).