Parlinski, Li, and Kawazoe Reply: In a recent Letter [1], we have calculated the soft mode in the cubic ZrO_2 using the standard CASTEP *ab initio* program [2], with the local-density approximation and pseudopotential approach, and confining the studied crystallite to a $2 \times 2 \times 2$ fcc supercell with periodic boundary conditions and 96 atoms. The force constants were directly derived from Hellmann-Feynman (HF) forces induced by separate Zr and O atomic displacements. Detraux, Ghosez, and Gonze [3] commented that for ZrO_2 the Born effective charges are not vanishing, and therefore, they should lead to the splitting of the transverse (TO)–longitudinal (LO) optic infrared active mode in the neighborhood of the Γ point. Indeed, the CASTEP program disregards the $\mathbf{k} = 0$ terms in the wave vector summations, although these interactions might lead to nonanalytical behavior of the dynamical matrix close to the Γ point and to LO-TO splitting. In an approximate way one could take into account the neglected components by supplementing the dynamical matrix with an additional term [4], namely,

$$\mathcal{D}_{\alpha,\beta}(\mathbf{k};\mu\nu) = \mathcal{D}^{(o)}_{\alpha,\beta}(\mathbf{k};\mu\nu) + \frac{4\pi e^2}{V\epsilon_\infty\sqrt{M_\mu M_\nu}} \frac{[\mathbf{k}\cdot\mathbf{Z}^*(\mu)]_\alpha[\mathbf{k}\cdot\mathbf{Z}^*(\nu)]_\beta}{|\mathbf{k}|^2} \times \exp\{-2\pi i g\cdot[\mathbf{r}(\mu) - \mathbf{r}(\nu)]\}\exp(-\mathbf{k}^2/\rho^2), \quad (1)$$

where $\mathbf{k}$ is the wave vector within a Brillouin zone with the center at the reciprocal lattice vector $\mathbf{g}$; V stays for the volume of the primitive unit cell; M_μ, $\mathbf{r}_\mu$ are atomic masses and positions; $\mathcal{D}^{(o)}_{\alpha,\beta}(\mathbf{k};\mu\nu)$ is the approximate dynamical matrix calculated by the direct method from the HF forces of CASTEP. Here, ρ is a free parameter which suppresses the influences of the second term of Eq. (1) once $\mathbf{k}$ moves away from $\mathbf{k} = 0$. If we choose $\rho = 0.062$ Å^{-1}, then this term vanishes close to the zone boundary point $X = (\frac{1}{2a}, 0, 0)$, where the phonon frequencies are well reproduced by the direct method alone [1] [without the nonanalytical term of Eq. (1)]. Using the Born effective charge tensors $\mathbf{Z}^*_{Zr} = +5.74$, $\mathbf{Z}^*_O = -2.87$, and the dielectric constant $\epsilon_\infty = 5.75$ calculated by Detraux, Ghosez, and Gonze we have recalculated our phonon dispersions, and the result is shown in Fig. 1. At $\mathbf{k} = 0$, the LO phonon splits away to a higher frequency of 19.72 THz. The TO phonon and the Raman active mode have not been influenced by the second term of Eq. (1) and remain at 8.46 and 16.54 THz, respectively. Except for the LO branch close to the Γ point, all other phonon branches, including the *soft mode* which is responsible for the cubic to tetragonal phase transition, are *not* affected by the nonanalytical term of the dynamical matrix.

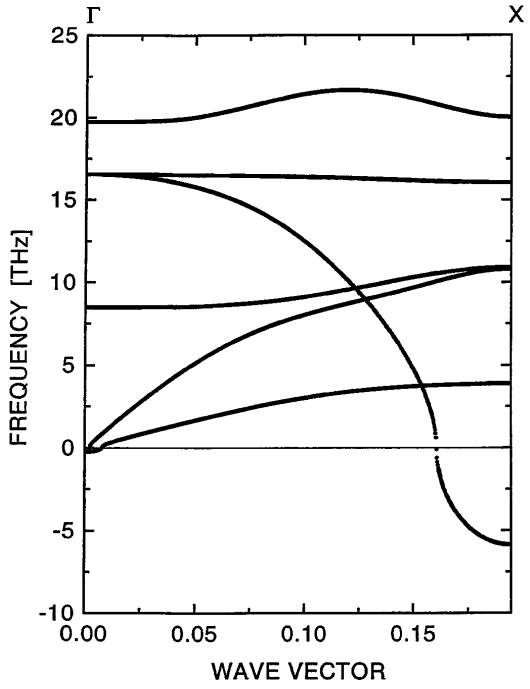

FIG. 1. Calculated phonon dispersions of ZrO_2 in the cubic phase with the nonanalytical term of the dynamical matrix, Eq. (1).

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