

AUTHOR CORRECTION **OPEN**



Author Correction: The elphbolt ab initio solver for the coupled electron-phonon Boltzmann transport equations

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Correction to: *npj Computational Materials* <https://doi.org/10.1038/s41524-022-00710-0>, published online 07 February 2022

The original version of this article contained typographical errors in Equation (6) and Equation (7).

The correct expression for Eq. (6) is

$$g_{\mathbf{k}\mathbf{q}}^{smn} = \sqrt{\frac{\hbar}{2m_r\hbar\omega_{s\mathbf{q}}}} \frac{1}{N_e N_{ph}} \sum_{\mathbf{R}_e \mathbf{R}_{ph}} \exp(i\mathbf{k} \cdot \mathbf{R}_e + i\mathbf{q} \cdot \mathbf{R}_{ph}) \times \sum_{s'm'n'} g_{\mathbf{R}_e \mathbf{R}_{ph}}^{s'm'n'} U_{nn'k'} U_{m'mk}^\dagger u_{s's\mathbf{q}} + g_{\mathbf{k}\mathbf{q}}^{Fr,smn}.$$

which replaces the previous incorrect version:

$$g_{\mathbf{k}\mathbf{q}}^{smn} = \sqrt{\frac{\hbar}{2m_r\hbar\omega_{s\mathbf{q}}}} \frac{1}{N_e N_{ph}} \sum_{\mathbf{R}_e \mathbf{R}_{ph}} \exp(i\mathbf{k} \cdot \mathbf{R}_e + i\mathbf{q} \cdot \mathbf{R}_{ph}) \times g_{\mathbf{R}_e \mathbf{R}_{ph}}^{smn} U_{nk'}^* U_{mk} u_{s\mathbf{q}} + g_{\mathbf{k}\mathbf{q}}^{Fr,smn}, \tag{6}$$

The correct expression for Eq. (7) is

$$g_{\mathbf{k}\mathbf{q}}^{Fr,smn} = i \frac{e^2}{\epsilon_0 V} \sum_{\tau} \sqrt{\frac{\hbar}{2m_r\hbar\omega_{s\mathbf{q}}}} [U_{k'} U_k^\dagger]_{nm} \sum_{\mathcal{G} \neq -\mathbf{q}} \frac{(\mathbf{q}+\mathcal{G}) \cdot \mathbf{Z}_\tau \cdot \boldsymbol{\xi}_{r,s\mathbf{q}}}{(\mathbf{q}+\mathcal{G}) \cdot \mathbf{e}^{\infty} \cdot (\mathbf{q}+\mathcal{G})} \times \exp[-i(\mathbf{q} + \mathcal{G}) \cdot \mathbf{r}_\tau].$$

which replaces the previous incorrect version:

$$g_{\mathbf{k}\mathbf{q}}^{Fr,smn} = i \frac{e^2}{\epsilon_0 V} \sum_{\tau} \sqrt{\frac{\hbar}{2m_r\hbar\omega_{s\mathbf{q}}}} U_{nk'}^* U_{mk} \sum_{\mathcal{G} \neq -\mathbf{q}} \frac{(\mathbf{q}+\mathcal{G}) \cdot \mathbf{Z}_\tau \cdot \boldsymbol{\xi}_{r,s\mathbf{q}}}{(\mathbf{q}+\mathcal{G}) \cdot \mathbf{e}^{\infty} \cdot (\mathbf{q}+\mathcal{G})} \times \langle nk' | \exp[-i(\mathbf{q} + \mathcal{G}) \cdot \mathbf{r}_\tau] | m\mathbf{k} \rangle, \tag{7}$$



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