Supplementary Material to the article

“Genesis of collective excitations in the conduction spectra of higher borides RB_6 and RB_{12} with cooperative structural instability”

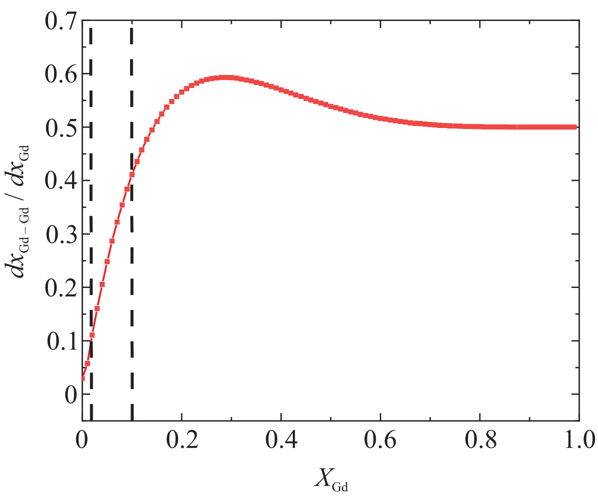

Fig. S1. The growth rate of the Gd-Gd pairs concentration with increasing x in the series $Gd_xLa_{1-x}B_6$. Vertical dotted lines show the range of compositions 2–10 % Gd (see text)

Estimation of the lattice contribution to the optical conductivity. To estimate the conductivity contribution from the lattice ions, we use the solution of Eq. (2) in the article for the coordinates of the ions, and the classical definition of the specific current

$$j_{\text{ion}} = q\dot{x}n_{\text{ion}}, \tag{S1}$$

where q is the ion charge and n_{ion} is the concentration of charged centers.

As a result, the lattice conductivity will have the form

$$\sigma_{\text{ion}} = \frac{2nq^2}{M}\frac{z\omega^2}{(\Omega^2-\omega^2)^2+4z^2\omega^2} \tag{S2}$$

(in (S2) we have retained the notation of formula (3) in the article). To calculate the contribution of ionic conductivity, it is necessary to estimate the ratio of ionic conductivity to the nonequilibrium correction $\frac{\sigma_{\text{ion}}}{\delta\sigma}$ obtained in the work in different spectral ranges. By direct substitution one can find

$$\frac{\sigma_{\text{ion}}}{\delta\sigma} = \frac{qmzc^2}{e^2Q}\frac{\omega^2(\gamma^2+\omega^2}{\gamma(\Omega^2-\omega^2)-2z\omega^2}, \tag{S3}$$

where the dipole parameter Q can be estimated from above as $Q = \frac{2kq}{a^3}$ (k is the conductivity coefficient in the Coulomb law for the SI system).

Using (S3) and the data of Table 1 of the article, we estimated the lattice contribution to the conductivity in various frequency intervals. For all the higher borides RB_6 and RB_{12} discussed in this work, the following results were obtained

$$\frac{\sigma_{\text{ion}}}{\delta\sigma}(\omega=\omega_0\sim 1\,\text{cm}^{-1}) \approx 10^{-10},$$

$$\frac{\sigma_{\text{ion}}}{\delta\sigma}(\omega=\omega_0\sim 500\,\text{cm}^{-1}) \approx 3\times 10^{-3},$$

$$\frac{\sigma_{\text{ion}}}{\delta\sigma}(\omega=\omega_0\sim 10000\,\text{cm}^{-1}) \approx 5\times 10^{-2}.$$

We note a very small value of the ionic contribution at low frequencies, which is explained by a sharp decrease in the ionic conductivity (dependence $\sigma_{\rm ion} \sim \omega^2$). Thus, the ionic conductivity in the systems under study in the entire frequency range below ω_{pl}, within the framework of the considered effects, turns out to be negligible and does not exceed 5 % even near the plasma edge.