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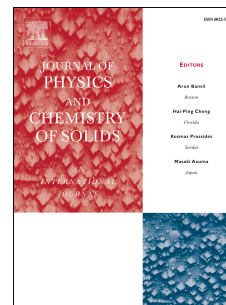
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Theoretical study of the local structures and the EPR parameters
for RLNKB glasses with VO²⁺ and Cu²⁺ dopants

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Abstract: The electron paramagnetic resonance (EPR) parameters and local structures for impurities VO²⁺ and Cu²⁺ in RO-Li₂O-Na₂O-K₂O-B₂O₃ (RLNKB; R = Zn, Mg, Sr and Ba) glasses are theoretically investigated by using the perturbation formulas of the EPR parameters for tetragonally compressed octahedral 3d¹ and tetragonally elongated octahedral 3d⁹ clusters, respectively. The VO²⁺ and Cu²⁺ dopants are found to undergo the tetragonal compression (characterized by the negative relative distortion ratios $\rho \approx -3\%$, -0.98% , -1% and -0.8% for R = Zn, Mg, Sr and Ba) and elongation (characterized by the positive relative distortion ratios $\rho \approx 29\%$, 17% , 16% and 28%), respectively, due to the Jahn-Teller effect. Both dopants show similar overall decreasing trends of cubic field parameter D_q and covalency factor N with decreasing electronegativity of alkali earth cation R. The conventional optical basicities Λ_{th} and local optical basicities Λ_{loc} are calculated for both systems, and the local Λ_{loc} are higher for Cu²⁺ than for VO²⁺ in the same RLNKB glass, despite the opposite relationship for the conventional Λ_{th} . This point is supported by the weaker covalency or stronger ionicity for Cu²⁺ than VO²⁺ in the same RLNKB system, characterized by the larger N in the former. The above comparative analysis on the spectral and local structural properties would be helpful to understand structures and spectroscopic properties for the similar oxide glasses with transition-metal dopants of complementary electronic configurations.

Keywords: RO-Li₂O-Na₂O-K₂O-B₂O₃; Electron paramagnetic resonance (EPR); Defect structures:
VO²⁺ and Cu²⁺

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