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Equilibrium Atomic Configurations Studies and Electron Paramagnetic Resonance of Binuclear Niobium Molecules in Li-Nb Phosphate Glass Dielectrics. SABRINA ARRINGTON-PEET, RAKHIM RAKHIMOV, VLADIMIR GAVRILENKO, Center of Materials Research, Norfolk State University, Norfolk VA 23504 — Equilibrium atomic configurations of binuclear niobium complexes Nb-O-Nb both free-standing and that embedded in lithium niobium phosphate glass (LNPG) are studied by total energy minimization method using *ab initio* pseudopotentials within density functional theory. Measurements of electron paramagnetic resonance revealed nonequivalent distribution of the charge and electron spin density between two Nb atoms. Measurements and theoretical analysis indicate that niobium atoms could exist in either of the two forms, Nb^{4+}-Nb^{4+} or Nb^{3+}-Nb^{5+}. The Nb atoms in freestanding molecule are equivalent with oxygen atom having only one local equilibrium position in the center of the molecule, indicating centro-symmetric structure. When the Nb complex is embedded into the glass the effect of external potential in LNPG resulted in an appearance of two non-equivalent configurations for the central oxygen atom in the molecule. Predicted nonequivalent geometries of the Nb-O-Nb complex embedded into LNPG is confirmed experimentally. Mechanism of the distortion is discussed.

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