

Nonlinear optical and phonon properties of NbOX₂ (X=Cl, Br, I)

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Abstract

We investigated the nonlinear optical processes and Raman response of two-dimensional ferroelectric materials NbOX₂ (X=Cl, Br, I). NbOX₂ exhibits stable in-plane ferroelectricity under atmospheric conditions and inversion symmetry breaking, resulting in strong second-order nonlinear processes. We observed that the intensity of second-harmonic generation (SHG) in reflection configuration increases with thickness below 30 nm and saturates around 50 nm. NbOX₂ displays five observable Raman modes, all belonging to the irreducible representation A of the C₂ group, as determined through polarization-resolved measurements. Our Raman measurements under uniaxial strain revealed anisotropic changes depending on the relative direction between the strain and Nb-O bond direction.