Stacking dependent ferroelectricity and antiferroelectricity in quasi-one-dimensional oxyhalides $NbOX_3$

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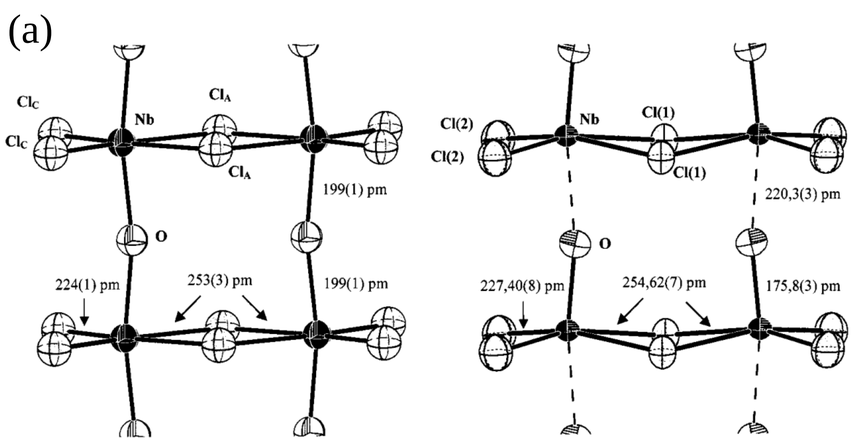
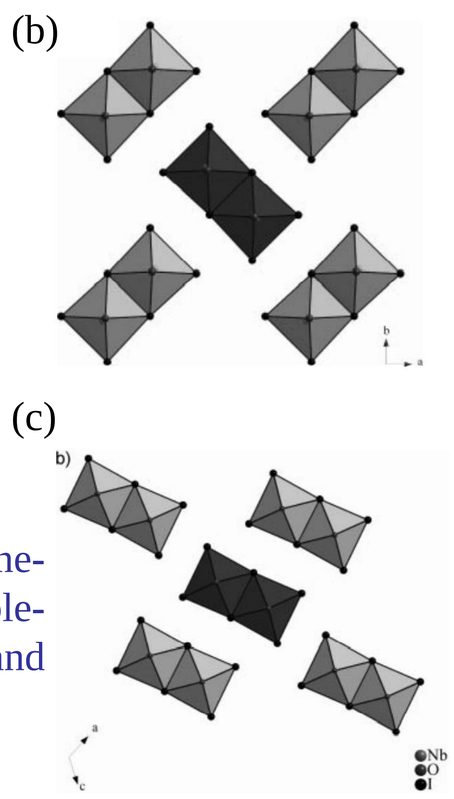
Low-dimensional ferroelectricity and polar materials have attracted considerable attentions for their fascinating physics and potential applications. Based on first-principles calculations, here we investigate the stacking modes and polar properties of a typical series of quasi-one-dimensional ferroelectrics: double-chain oxyhalides $NbOX_3$ (X=Cl, Br, I). The geometry of their double-chains allows both the interchain/intrachain permutation. Thus, different stacking modes of double-chains lead to a variety of ferroelectric and antiferroelectric phases in both the tetragonal and monoclinic crystals. The proximate energies of these phases may lead to multiphase coexistence in real materials, as well as the hydrostatic pressure driving structural phase transition. Their spontaneous polarizations and piezoelectricity of the ferroelectric phases are prominent, comparable to commercially used ferroelectric $BaTiO_3$ and piezoelectric ZnO, respectively. Our work demonstrates that the van der Waals $NbOX_3$ are promising materials for exploring quasi-one-dimensional ferroelectricity and antiferroelectricity

◎Background

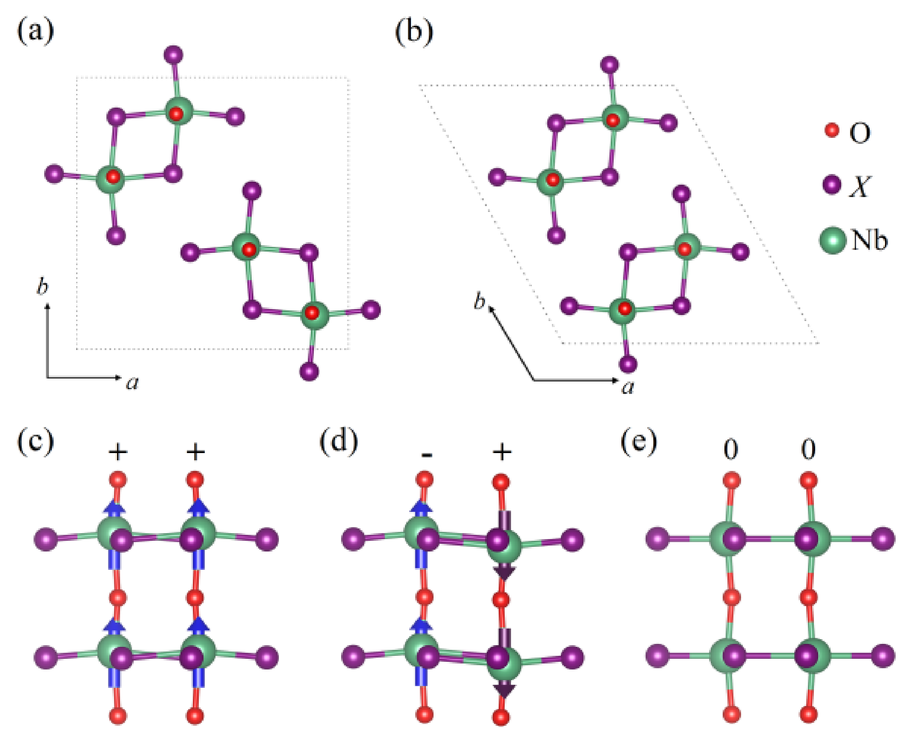




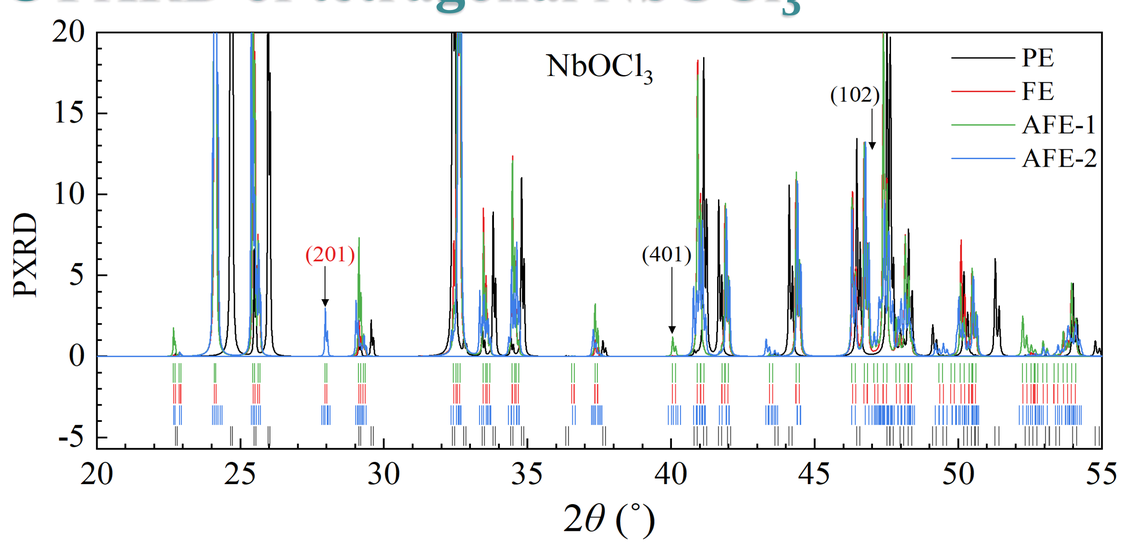
The structures of $NbOX_3$ bulk stacked by one-dimensional (1D) double-chains. (a) Two 1D double-chains of $NbOCl_3$. (b) and (c) are tetragonal and monoclinic crystal structures, respectively.

M. Ströbele et al, Z. Anorg. Allg. Chem. 628, 488 (2002).
S. Hartwig et al, Z. Anorg. Allg. Chem. 634, 115 (2008).

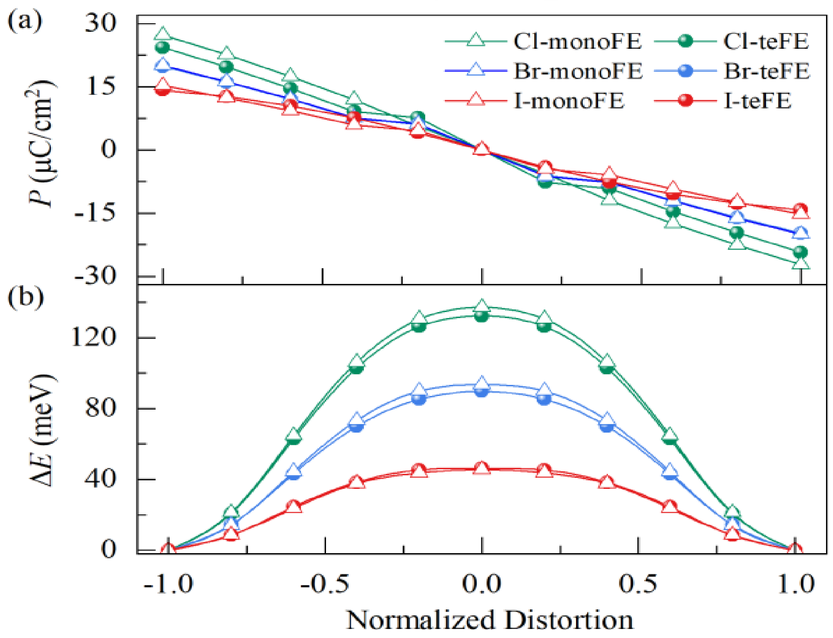
◎Structure



◎PXRD of tetragonal $NbOCl_3$



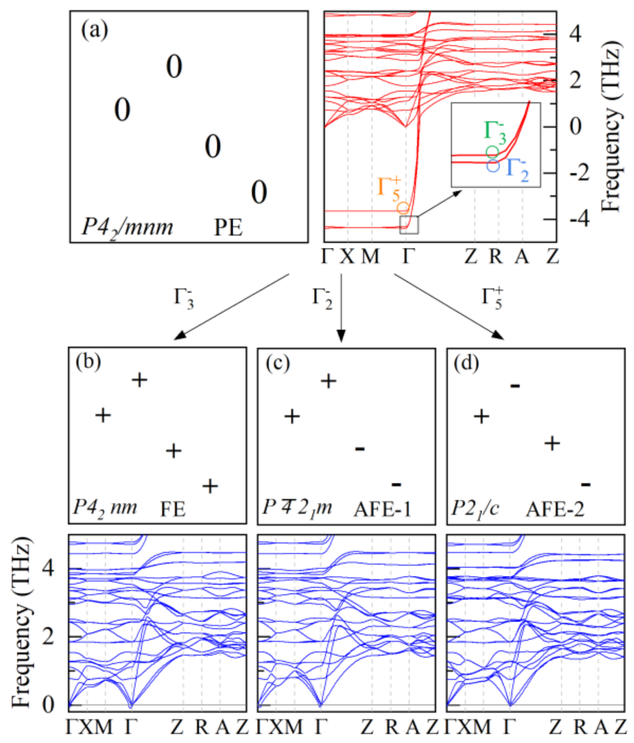
◎ Ferroelectricity & piezoelectricity



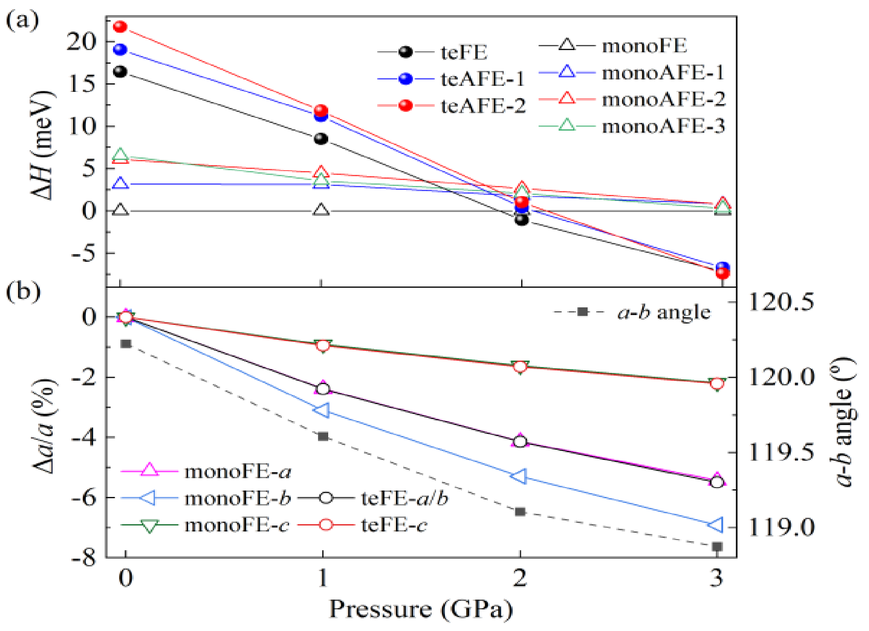
	phase	P(μC/cm²)	barrier(meV/f.u.)	d_{33}
$NbOCl_3$	moFE	27.2	34	
	teFE	24.3	33	34.6
$NbOBr_3$	moFE	20.0	23	
	teFE	19.8	22	36.9
$NbOI_3$	moFE	15.3	11	60.1
	teFE	14.2	12	

- Ferroelectric switching of $NbOX_3$ bulks
- The values of polarization, barrier and piezoelectric coefficient d_{33}

◎ Distortion modes & phonon spectra



◎ Phase evolution under pressure



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