Lattice dielectric properties of rutile TiO2 from first principles

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ルチル TiO2 の格子関数を非調和フォノンの理論を用いて計算した.

I. INTRODUCTION

- TiO2 の重要性
- TiO2 の研究の歴史
- フォノン非調和理論

II. THEORY

Frequency shift

lifetime

$$\mathrm{Im}\,\Sigma(\omega) = \mathrm{Im}\,\Sigma^{\mathrm{B}}[G_{\mathrm{NL}}, \Phi_3](\omega) \tag{1}$$
$$\gamma_{0j}^{4ph} = \mathrm{Im}\,\Sigma^{4ph}[G_{\mathrm{NL}}, \Phi_4](\omega = \Omega_{\mathrm{NL}}) \tag{2}$$

dielectric function

$$\epsilon_{\alpha\beta}(\omega) = \epsilon_{\alpha\beta}^{\infty} + \frac{1}{\Omega_0} \sum_{(0,j)} \frac{S_{\alpha\beta}^{j}}{\left(\Omega_{0j}^{\mathrm{NL}}\right)^2 - \omega^2 + i\Omega_{0j}^{\mathrm{NL}}\Sigma_{0j}^{\mathrm{B}}(\omega) + i\omega\gamma_{0j}^{4ph}} \tag{3}$$

III. RESULTS AND DISCUSSION

A. Computational Details

B. band structure

TABLE I. Calculated and reference structural parameters

	a [Å]	c [Å]	u	c/a	V [Å^3]
LDA	4.552	2.922	0.3038	0.642	
r2SCAN	4.602	2.961	0.3046	0.643	
exp 300K	4.5931	2.9589	0.30476	0.644	
X ray 298K	4.5937	2.9587	0.30511	0.644	
exp 15K	4.5867	2.9541	0.30469	0.644	

- バンド図 r2SCAN, harmonic vs scph+bubble3
- バンド図 LDA vs r2SCAN

TABLE II. Born Effective Charge

	a[Å]	c[Å]	u	c/a	V[Å^3]
LDA	4.552	2.922	0.3038	0.642	
r2SCAN	4.602	2.961	0.3046	0.643	
exp 300K	4.5931	2.9589	0.30476	0.644	
X ray 298K	4.5937	2.9587	0.30511	0.644	
exp 15K	4.5867	2.9541	0.30469	0.644	

C. lifetime and thermal conductivity

D. dielectric function

IV. CONCLUSIONS

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