Charge-Discharge Mechanism, Lithium-Ion Diffusion in Al, Ca, and Cu doped Lithium Meta Titanate based Anodes for Li-Ion Batteries: First Principle Study

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Computational details

The average voltage of LTO in regard to Li metal is represented by way of

$$V = -[E(Al-LTO) - E\left(Al-L_{1-x}TO\right) - E(Li)]/F \quad \text{----Eq.(S1)}$$

where E is the average energy of a completely stress-free ground-level structure, and F is the Faraday constant.

Single-electron oxidation voltage (V_{ox}) related to the Li^+/Li reference electrode was measured as follows:

$$V_{ox\,(vs.\,Li+/Li)} = -[E(Al-LTO) - E\left(Al-L_{1-x}TO\right) - E(Li)]/F + E_{SCE/SHE} - E_{(Li+/Li)SHE} \text{-Eq.(S2)}$$

where F is Faraday's constant. $E_{\circ\,\mathrm{SCE}/\mathrm{SHE}}$ (0.24) and $E_{\circ(\mathrm{Li}+/\mathrm{Li})/\mathrm{SHE}}$ (-3.04 V) are the potentials of an electron in a vacuum and of a metallic lithium electrode

Reduction potential is given as

$$V_{ox\,(vs.\,Li+/Li)} = -[E(Al-LTO) - E\left(Al-L_{1-x}TO\right) - E(Li)]/F - E_{(Li+/Li)SHE} \text{ -- Eq.(S3)}$$

where M′ = Mn, Fe, Ni, F is Faraday's constant. $E_{(\mathrm{Li}+/\mathrm{Li})/\mathrm{SCE}}$ (-3.04 V) are the potentials of metallic lithium with respect to saturated calomel electrode

The average volumetric energy density is expressed as

$$\Omega = -[E(Al-LTO) - E\left(Al-L_{1-x}TO\right) - E(Li)]/V_{average} \text{-----Eq.(S4)}$$

where $V_{average}$ is the average volume of the fully relaxed ground state structure.

The gravimetric energy density is proposed as

$$\gamma = -[E(Al-LTO) - E\left(Al-L_{1-x}TO\right) - E(Li)]/m_{average} \text{ ----Eq.(S5)}$$

where m_{av} is the average mass of a completely stress-free ground-level structure

The theoretical specific capacity of an anode material can be expressed by Faraday's law:

$$Q_{theoretical} = (nF/3600 * M_w)\ \text{mA h g}^{-1} \text{ ----Eq.(S6)}$$

Where n is the number of charge carriers, F is the Faraday constant, F=26.801×10^3 mA h mol^{-1} and Mw is the molecular weight of the active material [1, 4].

Results and discussion

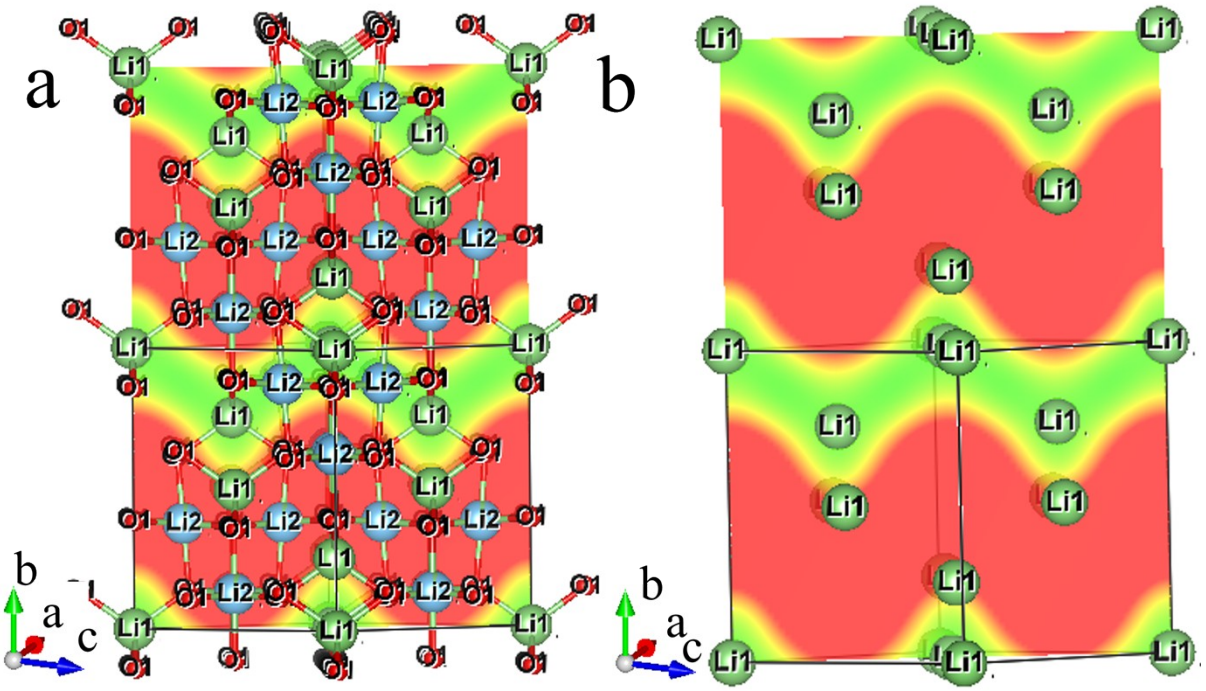

Figure 1. (a-b) Li-ion diffusion from CDD analysis along ac-plane.

Table S1. Total energies of Al, Ca, Cu-doped LTO.

Parameters	Al-LTO	Al-D-LTO	Al-TO
Total energy (eV)	-7699.050	-7488.591	-7490.63
	Ca-LTO	Ca-D-LTO	Ca-TO
	-15255.096	-15046.034	-14837.972
	Cu-LTO	Cu-D-LTO	Cu-D-TO
	-35171.849	-34962.419	-34096.716

Table S2 . Different thermal properties of considered configurations

Material	Internal energy(eV)	Entropy (J/K)	Enthalpy (eV)	Gibbs free energy (J)	a, Å	V (Å^3)
LTO	-103.319	19.318	-78.92	-5765.6	8.357, 90.00	583.65
D-LTO	-105.4749	22.594	-119.43	-6778.23		
D-TO	-99.15	37.725	-128.03	-11317.4		
Al-LTO	-769.869	13.807	-318.245	-4160.25	8.357, 90.00	583.65
Al-D-LTO	-769.81	21.86	-329.01	-6558.02		
Al-TO	681.86	22.478	-390.82	-6743.388		
Ca-LTO	-560.36	35.9175	-14531.57	10775.1	8.357, 90.00	583.65
Ca-D-LTO	-560.56	-41.5468	-14612.75	21464.04		
Ca-TO	-526.56	-45.063	-13419.66	13518.6		
Cu-LTO	-129.24	43.13	-34675.89	-12939.08	8.357, 90.00	583.65
Cu-D-LTO	-129.26	44.14	-34707.42	-13242		
Cu-TO	-125.3	95.436	-32938.56	-28630.8		

Thermal properties

Change in Gibbs free energy is given by

For Li-ion de-intercalation (charging) in Al-LTO

$\Delta G = G_{Al\text{-}D\text{-}LTO} - G_{Al\text{-}LTO} = -6558.02 - (-4160.25) = -2397.77$ J

$\Delta G < 0$ strong adsorption, exothermic, spontaneous process

The energy of -2397.77 J is useful for ejection of electron from cathode materials during charging

For Li-ion de-intercalation in Ca-LTO

$\Delta G = G_{Ca\text{-}D\text{-}LTO} - G_{Ca\text{-}LTO} = 21464.04 - (10775.1) = 10688.9$ J

$\Delta G > 0$ weak adsorption, endothermic

For Li-ion de-intercalation in Cu-LTO

$\Delta G = G_{Cu\text{-}D\text{-}LTO} - G_{Cu\text{-}LTO} = -13242 - (-12939.08) = 303$ J

$\Delta G < 0$ strong adsorption, exothermic

Mechanical properties

Various mechanical properties of $Li_4M_{2.5}Ti_{2.5}O_{12}$, $Li_2M_{2.5}Ti_{2.5}O_{12}$, and $M_{2.5}Ti_{2.5}O_{12}$ (M= Al, Ca, and Cu) that are elastic constants (C_{ij}), compliance (S_{ij}) calculated by adopting the DFT calculations [1-3]. Here we have considered a 6×6 symmetric matrix with 36 elements required to elaborate the stress and strain relationship.

$$\sigma_{ij} = \sum_{kl} C_{ijkl}\, \varepsilon_{kl} \quad \text{---Eq.(S7)}$$

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \tau_{yz} \\ \tau_{zx} \\ \tau_{xy} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \gamma_{yz} \\ \gamma_{zx} \\ \gamma_{xy} \end{pmatrix}$$

---------- Eq.(S8)

For the cubic system, elastic constants are reduced to 3. The strain dependence of stress can be elaborated as $C_{11} = C_{22} = C_{33}$, $C_{12} = C_{21} = C_{23} = C_{32} = C_{13} = C_{31}$, $C_{44} = C_{55} = C_{66}$ due to the fact that the *x*, *y*, and *z* axes are identical by symmetry. Also, the off-diagonal shear components are zero, i.e., $C_{45} = C_{54} = C_{56} = C_{65} = C_{46} = C_{64} = 0$, and mixed compression/shear coupling does not occur, i.e., $C_{14} = C_{41} = C_{51} = C_{15} = C_{61} = C_{16} = 0$. Therefore, the cubic elasticity matrix has the form of

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \tau_{yz} \\ \tau_{zx} \\ \tau_{xy} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \gamma_{yz} \\ \gamma_{zx} \\ \gamma_{xy} \end{pmatrix}$$

---------- Eq.(S9)

Where σ is the tensile stress, τ is the shear stress, ε is the tensile strain, and γ is the shear strain C_{ij} (i= 1, 6 j = 1, 6) are elastic constant matrix elements, and they are inversely related to compliance (S_{ij}) matrix element that can be expressed as

$$S_{ij} \propto 1/C_{ij}$$ --------Eq.(S10)

$$S_{ij} = K/C_{ij}$$ ------ Eq. (S11)

Where K is constant whose value is 0.0999 obtained from the DFT calculation[3].

Mechanical stability condition

Lattice mechanical stability and criteria for stability can be elaborated in terms of elastic constants C_{ij} [4]. Stability condition for the cubic crystal system can be expressed as

$$C_{11} - C_{12} > 0$$ ---------- Eq. (S12)

$$C_{11} + 2\,C_{12} > 0$$ ---------- Eq. (S13)

$$C_{11} > 0,\ C_{44} > 0$$ ---------- Eq. (S14)

$B_V = (2\,C_{11} + C_{11} + 2\,C_{12} + 4\,C_{12}) / 9 = (3\,C_{11} + 6\,C_{12}) / 9$ ---- Eq. (S15)

$G_V = (2\,C_{11} + C_{11} - C_{12} - 2\,C_{12} + 6\,C_{44} + 3\,C_{44}) /15$

$= (3\,C_{11} - 3\,C_{12} + 9\,C_{44}) / 15$ ----Eq. (S16)

B_R =10 / (2 S_{11} + S_{11} + 2 S_{12} + 4 S_{14}) = 10 / (3 S_{11} + 6 S_{12}) ----Eq. (S17)

1/G_R = (10 / 15) (4 (3 S_{11}) -4 (3 S_{14}) + 3 (S_{11}+2 S_{44})) ----Eq. (S18)

Bulk modulus (B) = (B_V + B_R) / 2 ----Eq. (S19)

Shear modulus (G) = (G_V + G_R) / 2 ----Eq. (S20)

Young modulus $(E) = 9\,B\,G/(3\,B + G\,)$----Eq. (S21)

B/G = ----Eq. (S22)

Poisson ratio $(\upsilon) = (3\,B - 2\,G)/(6\,B + 2\,G)$ ----Eq. (S23)

Shear anisotropic factor for the {100} shear planes between the ⟨011⟩ and ⟨010⟩ direction is

$$A_1 = 4\,C_{44} / (\,C_{11} + C_{33} - 2\,C_{13})$$----Eq. (S24)

Shear anisotropic factor for the {010} shear planes between the ⟨101⟩ and ⟨001⟩ direction is

$$A_2 = 4\,C_{55} / (\,C_{22} + C_{33} - 2\,C_{23})$$ ----Eq. (S25)

Shear anisotropic factor for the {001} shear planes between the ⟨110⟩ and ⟨010⟩ direction is

$$A_3 = 4\,C_{66} / (\,C_{11} + C_{22} - 2\,C_{12})$$ ----Eq. (S26)

Electrochemical properties of full cell graphite (Gr)/Al-LTO

DFT calculations of Gr/Al, Ca, Cu-LTO cell are given below

Average voltage of Gr/ Al, Ca, Cu-LTO cell,

$$V = -[E(Al-LTO) + E(C_6) - E(LiC_6) - E(Al-L_{1-x}TO)]/F$$ ----Eq.(S27)

Oxidation potential of Gr/ LTO cell

$$V_{ox\,(vs.\,Li+/LTO)} = -[E(LiC_6) - E(C_6)]/F + E_{SCE/SHE} - E_{(Li+/Li)SHE}$$ -Eq.(S28)

Reduction potential is given as

$$V_{ox\,(vs.\,Li+/LTO)} = -[E(LiC_6) - E(C_6)]/F + E_{SCE/SHE} - E_{(Li+/C_6)SCE}$$ -- Eq.(S29)

Gravimetric energy density of Gr/ LTO cell

$$\gamma = -[E(Al-LTO) + E(C_6) - E(LiC_6) - E(Al-L_{1-x}TO)]/m_{average}$$ ----Eq.(S30)

Volumetric energy density of Gr/ LTO cell

$$\gamma = -[E(Al-LTO) + E(C_6) - E(LiC_6) - E(Al-L_{1-x}TO)]/V_{average}$$ ----Eq.(S31)

where $V_{average}$ $m_{average}$ are the average volume of the fully relaxed ground state structure, average mass of a completely stress-free ground-level structure respectively.

Methods for elastic modulus

There are two methods to evolve the elastic modulus, the first is the Voigt scheme, and the second is the Reuss [3]. For orthorhombic crystals, the shear modulus (*G*) and bulk modulus (*B*) in accordance with Reuss (subscripts *R*) and Voigt (subscripts *V*) approximations are given by Substitute the values of C_{ij} and S_{ij} that are given below

Table S3.The elastic constants (C_{ij}), compliance (S_{ij}) of LTO.

Al-LTO	C_{11}	C_{44}	C_{12}
	125.68	120.75	105.49
	S_{11}	S_{44}	S_{12}
	0.00079488	0.00082733	0.000947
Al-D-LTO	C_{11}	C_{44}	C_{12}
	122.473	121.13	115.67
	S_{11}	S_{44}	S_{12}
	0.0008157	0.0008247	0.0008637
Al-TO	C_{11}	C_{44}	C_{12}
	89.99	80.934	76.39
	S_{11}	S_{44}	S_{12}
	0.001110	0.001234	0.001308

Ca-LTO	C_{11}	C_{44}	C_{12}
	66.98	62.59	60.789
	S_{11}	S_{44}	S_{12}
	0.00149	0.001596	0.00164
Ca-D-LTO	C_{11}	C_{44}	C_{12}
	59.895	54.69	53.74
	S_{11}	S_{44}	S_{12}
	0.001668	0.001827	0.001859
Ca-TO	C_{11}	C_{44}	C_{12}
	252.8	249.95	85.94
	S_{11}	S_{44}	S_{12}
	0.000395	0.0003997	0.001162
Cu-LTO	C_{11}	C_{44}	C_{12}
	164.03	137.17	64.69
	S_{11}	S_{44}	S_{12}
	0.00061	0.0007283	0.00154
Cu-D-LTO	C_{11}	C_{44}	C_{12}
	129.09	125.679	122.38
	S_{11}	S_{44}	S_{12}
	0.000774	0.000795	0.000816
Cu-D-TO	C_{11}	C_{44}	C_{12}
	322.5	320.197	207.58
	S_{11}	S_{44}	S_{12}
	0.00031	0.000312	0.00048

Al-LTO

$C_{11} - C_{12} > 0$, 125.68 -105.49 = 20.19 >0

$C_{11} + 2\ C_{12} > 0$, 125.68 + 2 (105.49) = 336.66 > 0

$C_{11} > 0$, $C_{44} > 0$, 125.68 > 0, 120.75 > 0

$B_V = (2\ C_{11} + C_{11} + 2\ C_{12} + 4\ C_{12}) / 9$

$= (3\ C_{11} + 6\ C_{12})/9 = (\ 3\ (125.68) + 6\ (105.49)\ ) / 9 = 112.22$

$G_V = (2\ C_{11} + C_{11} - C_{12} - 2\ C_{12} + 6\ C_{44} + 3\ C_{44}) /15$

$= (3\ C_{11} - 3\ C_{12} + 9\ C_{44}) / 15$

$G_V = (\ 3\ (125.68) -3\ (105.49) + 9\ (120.75)) / 15 = 76.488$

$B_R = 10 / (\ 2\ S_{11} + S_{11} + 2\ S_{12} + 4\ S_{14}) = 10 / (\ 3\ S_{11} + 6\ S_{12})$

= 10 / (3 (0.00079488) + 6 (0.000947))

= 10 / 0.00806664 = 1239.67352

$1/G_R = (10 / 15)\ (4\ (3\ S_{11}) -4\ (3\ S_{14}) + 3\ (S_{11}+2\ S_{44}))$ ----Eq. (S18)

= (10/15) (4 (3 (0.00079488)) - 4 (3 (0.000947)) + 3 ((0.00079488) + 2 (0.00082733)))

= (10/15) (0.00552318) = 0.00368212

G_R = 271.5827

Bulk modulus (B) = $(B_V + B_R) / 2$ = (112.22+1239.67352) / 2 = 675.95

Shear modulus (G) = $(G_V + G_R) / 2$ = (76.488+271.5827) / 2 = 174.03

Young modulus (E) = 9BG/(3B+G) = (9 (675.95) (174.03)) / (3 (675.95)+174.03) = 480.83

B/G = 675.95 / 174.03 = 3.88

Poisson ratio (υ) = (3B – 2G)/(6B+2G)

= (3 (675.95) – 2 (174.03)) / (6 (675.95) + 2 (174.03)) = 0.38

Shear anisotropic factor for the {100} shear planes between the ⟨011⟩ and ⟨010⟩ direction is

$$A_1 = 4C_{44}/(C_{11}+C_{33} -2C_{13})$$

$$= 4C_{44}/(2C_{11}-2C_{12}) = 4\ (120.75) / (2\ (125.68) - 2\ (105.49)) = 11.96$$

Shear anisotropic factor for the {010} shear planes between the ⟨101⟩ and ⟨001⟩ direction is

$$A_2 = 4C_{55}/(C_{22}+C_{33}-2C_{23})$$

$$A_2 = 4C_{44}/(2C_{11}-2C_{12}) = 4\ (120.75) / (2\ (125.68) -2\ (105.49)) = 11.96$$

Shear anisotropic factor for the {001} shear planes between the ⟨110⟩ and ⟨010⟩ direction is

$$A_3 =4C_{66}/(C_{11}+C_{22}-2C_{12})$$

$$A_3 = 4C_{44}/(2C_{11}-2C_{12}) = 4\ (120.75) / (2\ (125.68) -2\ (105.49)) = 11.96$$

Al-D-LTO

$C_{11} - C_{12} > 0$, 122.473-115.67= 6.8 >0

$C_{11} + 2\ C_{12} > 0$, 122.473+2 (115.67) = 353.81 > 0

$C_{11} > 0$, $C_{44} > 0$, 122.473 > 0, 121.13 > 0

$B_V = (2\ C_{11}+C_{11}+2\ C_{12}+4\ C_{12}) / 9 = (3\ C_{11} + 6\ C_{12}) / 9$

$= (3\ (122.473) + 6\ (115.67)) / 9 = 117.94$

$G_V = (2\ C_{11}+C_{11}-C_{12} -2\ C_{12} + 6\ C_{44} +3\ C_{44})/15$

$= (3\ C_{11} -3\ C_{12}+9\ C_{44}) / 15 = (3\ (122.473) -3\ (115.67) + 9\ (121.13)) / 15 = 74.04$

$B_R = 10 / (2\ S_{11}+S_{11}+2\ S_{12}+4\ S_{14})$

$= 10 / (3\ S_{11} + 6\ S_{12}) = 10 / (3\ (0.0008157)+6\ (0.0008637)) = 1310.7$

$1 / G_R = (10/15)\ (4\ (3\ S_{11}) - 4\ (3\ S_{12}) + 3\ (S_{11}+2\ S_{44}))$

$= (10/15)\ (4\ (3\ (0.0008157)) -4\ (3\ (0.0008637)) + 3\ ((0.0008157) + 2\ (0.0008247))$

$= 0.0343$

$1 / G_R = 0.0343$, $G_R = 29.155$

Bulk modulus (B) = (B_V + B_R) /2 = (117.94 +1310.7) /2 = 714.3

Shear modulus (G) = (G_V + G_R) / 2 = (74.04 +29.155) /2 = 51.598

Young modulus (E) = 9 B G/ (3 B+G)

= (9 (714.3) (51.598)) / (3 (714.3) + (51.598)) =151.15

B/G = 714.3/51.598 = 13.84

Poisson ratio (υ) = (3B – 2G)/(6B+2G)

= (3 (714.3) -2 (51.598)) / (6 (714.3) + 2 (51.598))

= 0.465

Shear anisotropic factor for the {100} shear planes between the ⟨011⟩ and ⟨010⟩ direction is

$A_1 = 4\ C_{44} / (\ C_{11} + C_{33} - 2\ C_{13})$

$= 4\ C_{44} / (2\ C_{11} - 2\ C_{12}) = 4\ (121.13) / (2\ (122.473) – 2\ (115.67)) = 35.61$

Shear anisotropic factor for the {010} shear planes between the ⟨101⟩ and ⟨001⟩ direction is

$A_2 = 4\ C_{55}/(C_{22}+C_{33}-2\ C_{23})$

$= 4\ C_{44} / (2\ C_{11} - 2\ C_{12}) = 4\ (121.13) / (2\ (122.473) – 2\ (115.67)) = 35.61$

Shear anisotropic factor for the {001} shear planes between the ⟨110⟩ and ⟨010⟩ direction is

$A_3 = 4\ C_{66} / (C_{11} + C_{22} - 2\ C_{12})$

For cubic system, $A_3 = 4\ C_{44} / (2\ C_{11} - 2\ C_{12})$

$= 4\ (121.13) / (\ 2\ (122.473) - 2\ (115.67)) = 35.61$

Al-TO

$C_{11} - C_{12} > 0,\ 89.99 - 76.39 = 13.6 > 0$

$C_{11} + 2\ C_{12} > 0,\ 89.99 + 2\ (76.39) = 242.77 > 0$

$C_{11} > 0,\ C_{44} > 0,\ 89.99 > 0,\ 80.934 > 0$

$B_V = (2\ C_{11} + C_{11} + 2\ C_{12} + 4\ C_{12}) / 9 = (3\ C_{11} + 6\ C_{12}) / 9$

$= (\ 3\ (89.99) + 6\ (76.39)) / 9 = 80.92$

$G_V = (2\ C_{11} + C_{11} - C_{12} - 2\ C_{12} + 6\ C_{44} + 3\ C_{44}) / 15$

$= (3\ C_{11} - 3\ C_{12} + 9\ C_{44}) / 15 = (3\ (89.99) - 3\ (76.39) + 9\ (80.934)) /15 = 51.28$

$B_R = 10 / (2\ S_{11} + S_{11} + 2\ S_{12} + 4\ S_{14}) = 10 / (3\ S_{11} + 6\ S_{12})$

$= 10/(3\ (0.001110) + 6\ (0.001308)) = 894.6$

$1/G_R = (10 / 15)\ (4\ (3\ S_{11}) - 4\ (3\ S_{12}) + 3\ (S_{11} + 2\ S_{44}))$

$= (10 / 15)\ (4\ (3\ (0.001110)) - 4\ (3\ (0.001308)) + 3\ ((0.001110) + 2\ (0.001234)))$

$= (10/15)\ (0.056136 - 0.015696) = 0.02696$

$G_R = 38.02$

Bulk modulus (B) = $(B_V + B_R) / 2 = (80.92 + 894.6) / 2 = 487.76$

Shear modulus (G) = $(G_V + G_R)/ 2 = (51.28 + 38.02) / 2 = 44.65$

Young modulus (E) = $9\ B\ G / (3\ B + G)$

$= (9\ (487.76)\ (44.65)) / (3\ (487.76) + (44.65)) = 129.98$

B/G = 487.76/44.65 = 10.92

Poisson ratio (υ) = $(3\ B - 2\ G) / (6\ B + 2\ G)$

$= (3\ (487.76) - 2\ (44.65)) / (6\ (487.76) + 2\ (44.65)) = 0.456$

Shear anisotropic factor for the {100} shear planes between the ⟨011⟩ and ⟨010⟩ direction is

$A_1 = 4\ C_{44} / (C_{11} + C_{33} - 2\ C_{13})$

$= 4\ C_{44} / (2\ C_{11} - 2C_{12}) = (4\ (80.934)) / (2\ (89.99) - 2\ (76.39)) = 11.90$

Shear anisotropic factor for the {010} shear planes between the ⟨101⟩ and ⟨001⟩ direction is

$A_2 = 4\ C_{55} / (C_{22} + C_{33} - 2\ C_{23})$

$= 4\ C_{44} / (2\ C_{11} - 2\ C_{12}) = (4\ (80.934)) / (2\ (89.99) - 2\ (76.39)) = 11.90$

Shear anisotropic factor for the {001} shear planes between the ⟨110⟩ and ⟨010⟩ direction is

$A_3 = 4\ C_{66} / (C_{11} + C_{22} - 2\ C_{12})$

$= 4\ C_{44} / (2\ C_{11} - 2\ C_{12})$

$$= (4\ (80.934)) / (2\ (89.99) - 2\ (76.39)) = 11.90$$

Ca-LTO

$C_{11} - C_{12} > 0$, $66.98-60.789 = 6.19 > 0$

$C_{11} + 2\ C_{12} > 0$, $66.98+2(60.789) = 188.6 > 0$

$C_{11} > 0$, $C_{44} > 0$, $66.98 > 0$, $60.789 > 0$

$B_V = (2\ C_{11} + C_{11} + 2\ C_{12} + 4\ C_{12}) / 9 = (3\ C_{11} + 6\ C_{12}) / 9 = (3(66.98)+6(60.789))/9 = 62.85$

$G_V = (2\ C_{11} + C_{11} - C_{12} - 2\ C_{12} + 6\ C_{44} + 3\ C_{44}) / 15$

$= (3\ C_{11} - 3\ C_{12} + 9\ C_{44}) / 15 = (3\ (66.98) - 3\ (60.789) + 9\ (60.789)) / 15 = 37.711$

$B_R = 10/(2\ S_{11} + S_{11} + 2\ S_{12} + 4\ S_{14})$

$= 10/(3\ S_{11}+6\ S_{12}) = 10 / (3\ (0.00149) + 6\ (0.00164)) = 698.81$

$1/G_R = (10/15)\ (4\ (3\ S_{11}) - 4\ (3\ S_{12}) + 3\ (S_{11}+2\ S_{44}))$

$= (10/15)\ (4\ (3\ S_{11}) - 4\ (3\ S_{12}) + 3\ (S_{11}+ 2\ S_{44}))$

$= (10/15)\ (4\ (3(0.00149)) - 4\ (3(0.00164)) + 3\ ((0.00149) + 2\ (0.001596))$

$= (10/15)\ (0.012246) = 0.008164$

$G_R = 122.459$

Bulk modulus (B) = $(B_V + B_R) / 2 = (62.85 + 698.81)/2 = 380.83$

Shear modulus (G) = $(G_V + G_R) / 2 = (37.711 + 122.459)/2 = 80.085$

Young modulus (E) = $9\ B\ G\ /(3\ B + G)$

$= (9\ (380.83)\ (80.085)) / (3\ (380.83) + (80.085)) = 224.52$

B/G = 380.83/80.085 = 4.76

Poisson ratio (υ) = $(3\ B - 2\ G) / (6\ B + 2\ G)$

$= (3\ (380.83) - 2\ (80.085)) / (6\ (380.83) + 2\ (80.085)) = 0.40$

Shear anisotropic factor for the {100} shear planes between the ⟨011⟩ and ⟨010⟩ direction is

$A_1 = 4\ C_{44} / (C_{11} + C_{33} - 2\ C_{13})$

$= 4\ C_{44} / (2\ C_{11} - 2\ C_{12})$

$= 4\ (62.59) / (2\ (66.98) - 2\ (60.789)) = 20.22$

Shear anisotropic factor for the {010} shear planes between the ⟨101⟩ and ⟨001⟩ direction is

$$A_2 = 4\,C_{55} / (\,C_{22} + C_{33} - 2\,C_{23})$$

$$A_2 = 4\,C_{44} / (2\,C_{11} - 2\,C_{12})$$

$$= 4\,(62.59) / (2\,(66.98) - 2\,(60.789)) = 20.22$$

Shear anisotropic factor for the {001} shear planes between the ⟨110⟩ and ⟨010⟩ direction is

$$A_3 = 4\,C_{66} / (C_{11} + C_{22} - 2\,C_{12})$$

$$A_3 = 4\,C_{44} / (2\,C_{11} - 2\,C_{12})$$

$$= 4\,(62.59) / (2\,(66.98) - 2\,(60.789)) = 20.22$$

Ca-D-LTO

$$C_{11} - C_{12} > 0,\ 59.895 - 53.74 = 6.155 > 0$$

$$C_{11} + 2\,C_{12} > 0,\ 59.895 + 2\,(53.74) = 167.36 > 0$$

$$C_{11} > 0,\ C_{44} > 0,\ 59.895 > 0,\ 54.69 > 0$$

$$B_V = (2\,C_{11} + C_{11} + 2\,C_{12} + 4\,C_{12}) / 9$$

$$= (3\,C_{11} + 6\,C_{12}) / 9 = (3\,(59.895) + 6\,(53.74)) / 9 = 55.792$$

$$G_V = (2\,C_{11} + C_{11} - C_{12} - 2\,C_{12} + 6\,C_{44} + 3\,C_{44}) / 15$$

$$= (3\,C_{11} - 3\,C_{12} + 9\,C_{44}) / 15$$

$$= (3\,(59.895) - 3\,(53.74) + 9\,(54.69)) / 15 = 34.045$$

$$B_R = 10 / (2\,S_{11} + S_{11} + 2\,S_{12} + 4S_{14})$$

$$= 10/(3S_{11}+6S_{12}) = 10 / (3\,(0.001668) + 6\,(0.001859)) = 618.89$$

$$1/G_R = (10/15)\,(4\,(3S_{11}) - 4\,(3\,S_{12}) + 3\,(S_{11}+2\,S_{44}))$$

$$= (10/15)\,(4\,(3\,(0.001668)) - 4\,(3\,(0.001859)) + 3\,((0.001668) + 2\,(0.001827))$$

$$= (10/15)\,(0.013674) = 0.009116$$

G_R = 109.697

Bulk modulus (B) = $(B_V + B_R)/2$ = (55.792+618.89) / 2 = 337.341

Shear modulus (G) = $(G_V + G_R)/2$ = (34.045 +109.697) / 2 = 71.87

Young modulus (E) = 9 B G/ (3 B+G)

= (9 (337.341) (71.87)) / (3 (337.341) + (71.87)) = 201.31

B/G = 337.341/71.87 = 4.694

Poisson ratio (υ) = (3 B – 2 G) / (6 B + 2 G)

= (3 (337.341) – 2 (71.87)) / (6 (337.341) + 2 (71.87)) = 0.4

Shear anisotropic factor for the {100} shear planes between the ⟨011⟩ and ⟨010⟩ direction is

$A_1 = 4\ C_{44} / (C_{11} + C_{33} - 2\ C_{13})$

$= 4\ C_{44} / (2\ C_{11} - 2\ C_{12})$

= (4(54.69)) / (2 (59.895) – 2 (53.74)) = 17.77

Shear anisotropic factor for the {010} shear planes between the ⟨101⟩ and ⟨001⟩ direction is

$A_2 = 4\ C_{55} / (C_{22} + C_{33} – 2\ C_{23})$

$A_2 = 4\ C_{44} / (2\ C_{11} – 2\ C_{12})$

= (4 (54.69)) / (2 (59.895) – 2 (53.74)) = 17.77

Shear anisotropic factor for the {001} shear planes between the ⟨110⟩ and ⟨010⟩ direction is

$A_3 = 4\ C_{66} / (C_{11} + C_{22} – 2\ C_{12})$

$A_3 = 4\ C_{44} / (2\ C_{11} – 2\ C_{12})$

= (4 (54.69)) / (2 (59.895) – 2 (53.74)) = 17.77

Ca-TO

$C_{11} - C_{12} > 0$, 252.8-85.94 = 166.86 >0

$C_{11} + 2\ C_{12} > 0$, 252.8+2(85.94) = 424.68 > 0

$C_{11} > 0$, $C_{44} > 0$, 252.8 > 0, 249.95 > 0

$B_V = (2\ C_{11} + C_{11} + 2\ C_{12} + 4\ C_{12}) / 9 = (3\ C_{11} + 6\ C_{12})/ 9$ = (3 (252.8) + 6 (85.94)) / 9

$= 141.56$

$G_V = (2\ C_{11} + C_{11} - C_{12} - 2\ C_{12} + 6\ C_{44} + 3\ C_{44})/15 =$

$= (3\ C_{11} - 3\ C_{12} + 9\ C_{44})\ /15$

$= (3\ (252.8) - 3\ (85.94) + 9\ (249.95))\ /\ 15 = 183.34$

$B_R = 10/(2\ S_{11} + S_{11} + 2\ S_{12} + 4\ S_{14})$

$= 10\ /\ (3\ S_{11} + 6\ S_{12}) = 10/\ (3\ (0.000395) + 6\ (0.001162)) = 1225.9$

$1/G_R = (10/15)\ (4\ (3\ S_{11}) - 4\ (3\ S_{12}) + 3\ (S_{11} + 2\ S_{44}))$

$= (10/15)\ (12\ (0.000395) - 12\ (0.001162) + 3\ ((0.000395) + 2\ (0.0003997)) = 0.00375$

$G_R = 266.67$

Bulk modulus (B) = $(B_V + B_R) / 2 = (141.56 + 1225.9) / 2 = 683.73$

Shear modulus (G) = $(G_V + G_R) / 2 = (183.34 + 266.67)/2 = 225$

Young modulus (E) = $9\ B\ G/(3\ B+G) = (9\ (683.73)\ (225))/\ (3\ (683.73) + (\ 225)) = 608.427$

B/G = 683.73/225 = 3.04

Poisson ratio (υ) = $(3\ B - 2\ G)\ /\ (6\ B + 2\ G)$

$= (3\ (683.73) - 2\ (225))\ /\ (6\ (683.73) + 2\ (225))$

$= 0.35$

Shear anisotropic factor for the {100} shear planes between the ⟨011⟩ and ⟨010⟩ direction is

$A_1 = 4\ C_{44}\ /(\ C_{11} + C_{33} - 2\ C_{13})$

$= 4\ C_{44}\ /(\ 2\ C_{11} - 2\ C_{12}) = (4\ (249.95))\ /\ (2\ (252.8)\ -2\ (85.94)) = 2.996$

Shear anisotropic factor for the {010} shear planes between the ⟨101⟩ and ⟨001⟩ direction is

$A_2 = 4\ C_{55}/\ (C_{22} + C_{33}\ -2\ C_{23})$

$= 4\ C_{44}/(2\ C_{11} - 2\ C_{12}) = (4\ (249.95))\ /\ (2\ (252.8) - 2\ (85.94)) = 2.996$

Shear anisotropic factor for the {001} shear planes between the ⟨110⟩ and ⟨010⟩ direction is

$A_3 = 4\ C_{66}/(C_{11} + C_{22} - 2\ C_{12})$

$= 4\ C_{44}/(2\ C_{11} - 2\ C_{12}) = (4\ (249.95))\ /(2\ (252.8) - 2\ (85.94))$

$= 2.996$

Cu-LTO

$C_{11} - C_{12} > 0,\ 164.03 - 64.69 = 99.34 > 0$

$C_{11} + 2\ C_{12} > 0,\ 164.03 + 2\ (64.69) = 293.41 > 0$

$C_{11} > 0,\ C_{44} > 0,\ 164.03 > 0,\ 137.17 > 0$

$B_V = (2\ C_{11} + C_{11} + 2\ C_{12} + 4\ C_{12})/\ 9 = (3\ C_{11} + 6\ C_{12})\ /\ 9$

$= (3\ (164.03) + 6\ (124.69))\ /\ 9 = 137.80$

$G_V = (2\ C_{11} + C_{11} - C_{12} - 2\ C_{12} + 6\ C_{44} + 3\ C_{44})/15$

$= (3\ C_{11} - 3\ C_{12} + 9\ C_{44})/15$

$= (3\ (164.03) - 3\ (124.69) + 9\ (137.17))\ /\ 15 = 90.17$

$B_R = 10\ /\ (2\ S_{11} + S_{11} + 2\ S_{12} + 4\ S_{14})$

$= 10\ /\ (3\ S_{11} + 6\ S_{12}) = 10\ /\ (3\ (0.00061) + 6\ (0.00080)) = 1508.3$

$1/G_R = (10\ /\ 15)\ (4\ (3\ S_{11}) - 4\ (3\ S_{12}) + 3\ (S_{11} + 2\ S_{44}))$

$= (10\ /\ 15)\ (12\ (0.00061) - 12\ (0.00080) + 3\ (0.00061 + 2\ (0.0007283)) = 0.0039198$

$G_R = 255.16$

Bulk modulus (B) = $(B_V + B_R)/2 = (137.80+1508.3)/2 = 823.05$

Shear modulus (G) = $(G_V + G_R)/2 = (90.17+255.16)/2 = 799.235$

Young modulus (E) = $9\ B\ G\ /\ (3\ B + G) = (9\ (823.05)\ (799.235))\ /\ (3\ (823.05) + (799.235))$

$= 1811.38$

B/G = 823.05/799.235 = 1.03

Poisson ratio (υ) = $(3\ B - 2\ G)\ /\ (6\ B + 2\ G)$

$= (3\ (823.05) - 2\ (799.235))\ /\ (6\ (823.05) + 2\ (799.235)) = 0.133$

Shear anisotropic factor for the {100} shear planes between the ⟨011⟩ and ⟨010⟩ direction is

$$A_1 = 4\,C_{44} / (C_{11} + C_{33} - 2\,C_{13})$$

$$= 4\,C_{44} / (2\,C_{11} - 2\,C_{12}) = (4\,(137.17)) / (2\,(164.03) - 2\,(124.69)) = 6.97$$

Shear anisotropic factor for the {010} shear planes between the ⟨101⟩ and ⟨001⟩ direction is

$$A_2 = 4\,C_{55} / (C_{22} + C_{33} - 2C_{23})$$

$$= 4\,C_{44} / (2\,C_{11} - 2\,C_{12})$$

$$= (4\,(137.17)) / (2\,(164.03) - 2\,(124.69)) = 6.97$$

Shear anisotropic factor for the {001} shear planes between the ⟨110⟩ and ⟨010⟩ direction is

$$A_3 = 4\,C_{66} / (C_{11} + C_{22} - 2\,C_{12})$$

$$= 4\,C_{44} / (2\,C_{11} - 2\,C_{12})$$

$$= (4\,(137.17)) / (2\,(164.03) - 2\,(124.69)) = 6.97$$

Cu-D-LTO

$C_{11} - C_{12} > 0$, $129.09 - 122.38 = 6.71 > 0$

$C_{11} + 2\,C_{12} > 0$, $129.09 + 2(122.38) = 373.82 > 0$

$C_{11} > 0$, $C_{44} > 0$, $129.09 > 0$, $122.38 > 0$

$$B_V = (2\,C_{11} + C_{11} + 2\,C_{12} + 4\,C_{12}) / 9 = (3\,C_{11} + 6\,C_{12}) / 9$$

$$= (3\,(129.09) + 6\,(122.38)) / 9 = 124.62$$

$$G_V = (2\,C_{11} + C_{11} - C_{12} - 2\,C_{12} + 6\,C_{44} + 3\,C_{44}) / 15$$

$$= (3\,C_{11} - 3\,C_{12} + 9\,C_{44}) / 15 = (3\,(129.09) - 3\,(122.38) + 9\,(125.679)) / 15 = 76.75$$

$$B_R = 10 / (2\,S_{11} + S_{11} + 2\,S_{12} + 4\,S_{14}) = 10 / (3\,S_{11} + 6\,S_{12})$$

$$= 10 / (3\,(0.000774) + 6\,(0.000816)) = 1385.4$$

$$1/G_R = (10/15)\,(4\,(3\,S_{11}) - 4\,(3\,S_{12}) + 3\,(S_{11} + 2\,S_{44}))$$

$$= (10/15)\,(12\,(S_{11}) - 12\,(S_{12}) + 3\,(S_{11} + 2\,S_{44}))$$

$$= (10/15)\,(12\,(0.000774) - 12\,(0.000816) + 3\,((0.000774) + 2\,(0.000795))$$

$$= (10/15)\,(0.006588) = 0.004392$$

$$G_R = 227.687$$

Bulk modulus (B) = $(B_V + B_R)/2$ = (124.62+1385.4)/2 = 755.01

Shear modulus (G) = $(G_V + G_R)/2$ = (76.75+227.687)/2 = 152.22

Young modulus (E) = 9 B G /(3 B + G)

= (9 (755.01) (152.22)) / (3 (755.01) + (152.22)) = 427.9

B/G = 755.01/152.22 = 4.96

Poisson ratio (υ) = (3 B – 2 G) / (6 B + 2 G)

= (3 (755.01) – 2 (152.22)) / (6(755.01) + 2 (152.22)) = 0.406

Shear anisotropic factor for the {100} shear planes between the ⟨011⟩ and ⟨010⟩ direction is

$A_1 = 4\ C_{44} / (\ C_{11} + C_{33} - 2\ C_{13})$

$= 4\ C_{44} /(2\ C_{11} – 2\ C_{12})$

= (4 (125.679)) / (2 (129.09) – 2 (122.38)) = 37.5

Shear anisotropic factor for the {010} shear planes between the ⟨101⟩ and ⟨001⟩ direction is

$A_2 = 4\ C_{55} /(\ C_{22} + C_{33} – 2\ C_{23})$

$= 4\ C_{44} /(\ 2\ C_{11} – 2\ C_{12})$

= (4 (125.679)) / (2 (129.09) – 2 (122.38)) = 37.5

Shear anisotropic factor for the {001} shear planes between the ⟨110⟩ and ⟨010⟩ direction is

$A_3 = 4\ C_{66} / (C_{11} + C_{22} – 2\ C_{12})$

$= 4\ C_{44} / (2\ C_{11} – 2\ C_{12})$ = (4 (125.679)) / (2 (129.09) – 2 (122.38))

= 37.5

Cu-TO

$C_{11} - C_{12} > 0$, 322.5 - 207.58 = 114.92 >0

$C_{11} + 2\ C_{12} > 0$, 322.5 + 2 (207.58) = 737.66 > 0

$C_{11} > 0$, $C_{44} > 0$, 322.5 > 0, 320.197 > 0

$B_V = (2\ C_{11} + C_{11} + 2\ C_{12} + 4\ C_{12})/ 9 = (3\ C_{11} + 6\ C_{12})/ 9$

= (3 (322.5) + 6 (207.58))/ 9 = 245.89

$G_V = (2\ C_{11} + C_{11} - C_{12} - 2\ C_{12} + 6\ C_{44} + 3\ C_{44})/15$

$= (3\ C_{11} - 3\ C_{12} + 9\ C_{44})/15 = (3\ (322.5) - 3\ (207.58) + 9\ (320.197))\ /\ 15 = 358.5$

$B_R = 10\ /\ (2\ S_{11} + S_{11} + 2\ S_{12} + 4\ S_{14}) = 10\ /\ (3\ S_{11} + 6\ S_{12})$

$= 10\ /\ (3\ (0.00031) + 6\ (0.00048)) = 2624.7$

$1/G_R = (10\ /\ 15)\ (4\ (3\ S_{11}) - 4\ (3\ S_{12}) + 3\ (S_{11} + 2\ S_{44}))$

$= (10\ /\ 15)\ (12\ (0.00031) - 12\ (0.00048) + 3\ (0.00031 + 2\ (0.000312)))$

$= (10/15)\ (0.000762) = 0.000508$

$G_R = 1968.5$

Bulk modulus (B) = $(B_V + B_R)/2 = (245.89+2624.7)\ /\ 2 = 1435.29$

Shear modulus (G) = $(G_V + G_R)/2 = (358.5+1968.5)\ /\ 2 = 1163.5$

Young modulus (E) = $9\ B\ G\ /(3\ B + G)$

$= (9\ (1435.29)\ (\ 1163.5))\ /\ (3\ (1435.29) + (\ 1163.5)) = 2747.96$

B/G = 1435.29/1163.5 = 1.23

Poisson ratio (υ) = $(3\ B - 2\ G)/(6\ B+2\ G)$

$= (3\ (1435.29) - 2\ (1163.5))\ /\ (6\ (1435.29) + 2\ (1163.5)) = 0.18$

Shear anisotropic factor for the {100} shear planes between the ⟨011⟩ and ⟨010⟩ direction is

$A_1 = 4\ C_{44}\ /\ (\ C_{11} + C_{33} - 2\ C_{13})$

$= 4\ C_{44}\ /(2\ C_{11} - 2\ C_{12}) = (4\ (320.197))/\ (2\ (322.5) - 2\ (207.58)) = 5.57$

Shear anisotropic factor for the {010} shear planes between the ⟨101⟩ and ⟨001⟩ direction is

$A_2 = 4\ C_{55}\ /(\ C_{22} + C_{33} - 2\ C_{23})$

$= 4\ C_{44}\ /(\ 2\ C_{11} - 2\ C_{12}) = (4\ (320.197))\ /\ (2(322.5) - 2\ (207.58)) = 5.57$

Shear anisotropic factor for the {001} shear planes between the ⟨110⟩ and ⟨010⟩ direction is

$A_3 = 4\ C_{66}\ /(\ C_{11} + C_{22} - 2\ C_{12})$

$= 4\ C_{44}\ /\ (2\ C_{11} - 2\ C_{12}) = (4\ (320.197))\ /\ (2\ (322.5) - 2\ (207.58))$

$= 5.57$

Electrochemical properties of half cell (Li/Al, Ca, Cu-LTO)

Al-LTO

The average voltage of LTO with respect to Li metal is represented as

$V = -[E(\text{Al-LTO}) - E(\text{Al-L}_{1-x}\text{TO}) - E(\text{Li})]/F$

where E is the average energy of fully relaxed ground state structure, F is the Faraday constant.

V=- [((-7699.051) - (-7488.592) - (-204.706)) eV] / (96.5 kJ/mol)

V= 4.75468 V ~ 4.8 V

Single-electron oxidation voltage (V_{ox}) related to the Li^+/Li reference electrode was measured as follows:

V_{ox} (vs. Li^+/Li) = [E (Al-LTO) − E(Al-L_{1-x}TO) – E (Li)] / F+ $E_{SCE\ /SHE} - E_{(Li+/Li)/SHE}$ Eqn. S19

where F is Faraday's constant. $E_{\circ\ SCE\ /SHE}$ (0.24) and $E_{\circ(Li+/Li)/SHE}$ (−3.04 V) are the potentials of an electron in a vacuum and of a metallic lithium electrode

V_{ox}(vs.Li+/Li)=[(-7699.051)-(-7488.592)-(-204.706)]/(96.5kJ/mol)+0.24-3.04 V

V_{ox}(vs.Li+/Li) = 4.75468 V +0.24-3.04 V = 1.955 V

Reduction potential is given as

V_{rx} (vs. Li^+/Li) = [E(Al-LTO) − E(Al-L_{1-x}TO)]/F − $E_{\circ(Li+/Li)/SCE}$

where M′ = Mn, Fe, Ni, F is Faraday's constant. $E_{(Li+/Li)/SCE}$ (-3.04 V) are the potentials of metallic lithium with respect to saturated calomel electrode

V_{rx}(vs.Li^+/Li)= [(-7699.051) - (-7488.592) - (-204.706)]/(96.5kJ/mol) -3.04 V

V_{rx} (vs. Li^+/Li) = 4.75468 V-3.04 V = 1.715 V

Average volumetric energy density is given as

$\Omega = -[E(\text{Al-LTO}) - E(\text{Al-L}_{1-x}\text{TO}) - E(\text{Li})]/V_{av}$

where Vav is the average volume of the fully relaxed ground state structure.

Ω = − [((-7699.051) - (-7488.592) - (-204.706)) eV] / (578.34×10^{-24} cm^3)

Ω = [4.75468x1.602×10^{-19} j]/(578.34×10^{-24} cm^3) [1eV=1.602×10^{-19} j],

[one joul (J) = 2.77778e-7 kW h]

Ω = [4.75468 x 1.602×10^{-19} x 2.77778e-7 kW h]/(578.34×10^{-24} cm^3)

Average volumetric energy density (Ω) = 0.36585 W h/cm^3

Average volumetric power density = 0.36585 W/cm^3

Specific energy is expressed as

$\gamma = -[E(Al\text{-}LTO) - E(Al\text{-}L_{1-x}TO) - E(Li)]/m_{av}$

where m_{av} is the average mass of a fully relaxed ground state structure

γ =−[((-7699.0510) - (-7488.592) - (-204.706)) eV]/(18.46372786 g/mol)

[4.75468x96.485kj/mole]/(18.46372786 g/mol)

[4.75468x96.485x2.77778 e-4 kW h]/(18.46372786 g)

= 6.901755195 Wh/g 1eV= 96.485kj/mole, kJ = 2.77778 e-4 kW h

Gravimetric energy density = 6.9 kWh/kg

Gravimetric power density = 6.9 kW/kg

Theoretical capacity

The theoretical capacity of a cathode material can be calculated by Faraday's law:

$Q_{theoretical} = (nF) / (3600*Mw)$ mA h g^{-1}

Where n is the number of charge carriers, F is the Faraday constant F=26.801×10^3 mA h $mol^{-1}$and Mw is the molecular weight of the active material.

$Q_{theoretical} = (1x26.801\times10^3)/(3.6*406.72135)$ mA h g^{-1}

= 183.04232 ~ 183.04 mA h g^{-1}

Al-D-LTO

The average voltage of LTO with respect to Li metal is represented as

$V = -[E(Al\text{-}L_{1-x}TO) - E(TO) - E(Li)]/F$

where E is the average energy of fully relaxed ground state structure, F is the Faraday constant.

V = − [(-7698.579) - (-7490.632) - (-204.706) eV)]/ 96.5 kJ/mol

V = 3.242122 V ~ 3.24 V

$Q_{theoretical}$ = (26.801×10^3 mA h) / (3.6 * 392.921345) mA h g^{-1}

= 189.47105 mA h g^{-1}

Al-D-TO

$Q_{theoretical}$ = (nF) / (3600*Mw) mA h g^{-1}

$Q_{theoretical}$ = (26.801×10^3 mA h) / (3.6*379.1213375) mA h g^{-1}

$Q_{theoretical}$ = 196.36779 ~ 196.4 mA h g^{-1}

Ca-LTO

The average voltage of LTO with respect to Li metal is represented as

V = − [E (Ca-LTO) – E (Ca-L_{1-x}TO) – E (Li)]/F

where E is the average energy of fully relaxed ground state structure, F is the Faraday constant.

V = − [((-15255.096) - (-15046.034) - (-204.706)) eV]/ 96.5 kJ/mol

V = [4.3560 eV] / 96.5 kJ/mol = 4.36 V

Single-electron oxidation voltage (V_{ox}) related to the Li^+/Li reference electrode was measured as follows:

V_{ox} (vs. Li+/Li) = [E(Ca-LTO) − E(Ca-L_{1-x}TO)]/F+ $E_{SCE\ /SHE}$ − $E_{(Li+/Li)/SHE}$

where F is Faraday's constant. $E_{\circ\ SCE\ /SHE}$ (0.24) and $E_{\circ(Li+/Li)/SHE}$ (−3.04 V) are the potentials of an electron in a vacuum and of a metallic lithium electrode

V_{ox} (vs. Li+/Li) = [(-15255.096) - (-15046.034) - (-204.706)]/ 96.5 kJ/mol+0.24V-3.04 V

= 4.36 V + 0.24 V - 3.04 V =1.56 V

Reduction potential is given as

V_{rx} (vs. Li^+/Li) = [E (Ca-LTO) – E (Ca-L_{1-x}TO)]/F − $E_{\circ(Li+/Li)/SCE}$

where M′ = Mn, Fe, Ni, F is Faraday's constant. $E_{(Li+/Li)/SCE}$ (-3.04 V) are the potentials of metallic lithium with respect to saturated calomel electrode

V_{ox} (vs. Li+/Li) = [(-15255.096) - (-15046.034) - (- 204.706)]/ 96.5 kJ/mol + 0.24V - 3.04 V

= 4.36 V-3.04 V =1.32 V

Average volumetric energy density is given as

Ω = − [E (Ca-LTO) – E (Ca-L_{1-x}TO) – E (Li)]/V_{av}

where Vav is the average volume of the fully relaxed ground state structure.

$\Omega = -[((-15255.096) - (-15046.034) - (-204.706))]/575.733 \times 10^{-24}\ cm^3$

$\Omega = -[4.35599\ eV]/ 575.733072 \times 10^{-24}\ cm^3$

$\Omega = -[4.35599 \times 1.602 \times 10^{-19} \times 2.77778e\text{-}7\ kW\ h]/ 575.733072 \times 10^{-24}\ cm^3$

$\Omega = 0.3366871\ W\ h/cm^3$ [1eV=1.602×10^{-19} j],

[one joul (J) = 2.77778e-7 kW h]

Average volumetric energy density = 0.3366871~0.337 W h/cm^3

Average volumetric power density = 0.3366871 ~ 0.337 W/cm^3

Specific energy is expressed as

$\gamma = -[E (Ca\text{-}LTO) - E (Ca\text{-}L_{1-x}TO) - E (Li)]/m_{av}$

where m_{av} is the average mass of a fully relaxed ground state structure

$\gamma = -[((-15255.096) - (-15046.034) - (-204.706))\ eV]/16.8074\ g/mol$

$\gamma = [4.355994265 \times 96.485 \times 2.77778\ e\text{-}4\ kW\ h/\sout{mol}]/(16.8073656\ g/\sout{mol})$

$\gamma = [6.94616825\ kW\ h/kg] \sim 6.95\ kW\ h/kg$

Gravimetric energy density = 6.95 kW h/kg

Gravimetric power density = 6.95 kW/kg

Theoretical capacity

The theoretical capacity of a cathode material can be calculated by Faraday's law:

$Q_{theoretical} = (nF) / (3600*Mw)\ mA\ h\ g^{-1}$

Where n is the number of charge carriers, F is the Faraday constant $F=26.801 \times 10^3$ mA h mol^{-1} and Mw is the molecular weight of the active material.

$Q_{theoretical} = (1 \times 26.801 \times 10^3) / (3.6 * 439.4625)\ mA\ h\ g^{-1}$

$Q_{theoretical} = 169.40517 \sim 169.4\ mA\ h\ g^{-1}$

Ca-D-LTO

The average voltage of Ca-D-LTO with respect to Li metal is represented as

$V = -[E (Ca\text{-}L_{1-x}TO) - E (Ca\text{-}TO) - E (Li)]/F$

V = − [(-15046.034) - (-14837.972) - (-204.706)]/ 96.5 kJ/mol

V = [3.35686882 V] ~ 3.4 V

$Q_{theoretical}$ = (nF) / (3600*Mw) mA h g^{-1}

$Q_{theoretical}$ = (1x26.801×10^3) /(3.6*425.6625) mA h g^{-1}

$Q_{theoretical}$ = 174.8973 mA h g^{-1}

Ca-D-TO

$Q_{theoretical}$ = (nF) / (3600*Mw) mA h g^{-1}

$Q_{theoretical}$ = (1x26.801×10^3)/(3.6*411.8625) mA h g^{-1}

$Q_{theoretical}$ = 180.75746 mA h g^{-1}

Cu-LTO

The average voltage of LTO with respect to Li metal is represented as

V = − [E (Cu-LTO) – E (Cu-L_{1-x}TO) – E (Li)]/F

where E is the average energy of fully relaxed ground state structure, F is the Faraday constant.

V =-[(-35171.849) - (-34962.4193) - (-204.706)]/96.5 kJ/mol

V = [4.724931104 V] ~ 4.7 V

Single-electron oxidation voltage (V_{ox}) related to the Li^+/Li reference electrode was measured as follows:

V_{ox} (vs. Li^+/Li) = [E (Cu-LTO) – E (Cu-L_{1-x}TO) – E (Li)]/F+ $E_{SCE\ /SHE}$ − $E_{(Li+/Li)/SHE}$

where F is Faraday's constant. $E_{\circ\ SCE\ /SHE}$ (0.24) and $E_{\circ(Li+/Li)/SHE}$ (−3.04 V) are the potentials of an electron in a vacuum and of a metallic lithium electrode

V_{ox}(vs.Li^+/Li) = [(-35171.849) - (-34962.4193) - (-204.706)]/ 96.5 kJ/mol + 0.24 -3.04 V

= 4.724931104 V + 0.24 V-3.04 V = 1.924931104 ~ 1.9 V

Reduction potential is given as

V_{rx} (vs. Li^+/Li) = [E (Cu-LTO) – E (Cu-L_{1-x}TO) – E (Li)]/F − $E_{\circ(Li+/Li)/SCE}$ Eqn. S20

where M′ = Mn, Fe, Ni, F is Faraday's constant. $E_{(Li+/Li)/SCE}$ (-3.04 V) are the potentials of metallic lithium with respect to saturated calomel electrode

V_{ox}(vs.Li^+/Li)=[(-35171.849) - (-34962.4193) - (-204.706)]/96.5 kJ/mol+0.24-3.04 V

= 4.72493 V-3.04 V = 1.684931104 ~ 1.7 V

Average volumetric energy density is given as

$\Omega = -$ [E (Cu-LTO) – E (Cu-L_{1-x}TO) – E (Li)]/V_{av} where Vav is the average volume of the fully relaxed ground state structure.

$\Omega = -$[(-35171.849) - (-34962.4193) - (-204.706)] / 575.0752027x$10^{-24}$$cm^3$

= [4.724931104 x 1.602×10^{-19} x 2.77778e-7 kW h]/575.0752027x$10^{-24}$$cm^3$

= 0.36561052 W h/ cm^3

Specific energy is expressed as

$\gamma = -$ [E (Cu-LTO) – E (Cu-L_{1-x}TO) – E (Li)]/m_{av} ----------(3)

where m_{av} is the average mass of a fully relaxed ground state structure

$\gamma = -$ [(-35171.849) - (-34962.419) - (-204.706)]/19.09597217g/mol

= [4.724931104 x 96.485 x 2.77778 e-4 kW h/~~mol~~]/ 19.09597217g/~~mol~~

= 6.631493604 kW h/kg

Gravimetric energy density = 6.631493604 kW h/kg ~ 6.6 kW h/kg

Gravimetric power density = ~ 6.6 kW/kg

Theoretical capacity

The theoretical capacity of a cathode material can be calculated by Faraday's law:

$Q_{theoretical}$ = (n F) / (3600*Mw) mA h g^{-1}

Where n is the number of charge carriers, F is the Faraday constant F=26.801×10^3 mA h $mol^{-1}$and Mw is the molecular weight of the active material.

$Q_{theoretical}$ = (1 x 26.801 × 10^3) / (3.6 * 498.1325) mA h g^{-1}

= 149.45265 mA h g^{-1}

$= 149.453 \text{ mA h g}^{-1}$

For Cu-D-LTO

The average voltage of LTO with respect to Li metal is represented as

$V = -[E(\text{Cu-L}_{1-x}\text{TO}) - E(\text{Cu-TO}) - E(\text{Li})]/F$

$V = -[(-34962.4193) - (-34096.716) - (-204.706)]/96.5 \text{ kJ/mol}$

$V = -[3.997523528 \text{ V}] = 4 \text{ V}$

$Q_{theoretical} = (1x26.801\times10^3) / (3.6*484.3325) \text{ mA h g}^{-1}$

$Q_{theoretical} = 149.45265 \text{ mA h g}^{-1}$

$Q_{theoretical} = 149.45 \text{ mA h g}^{-1}$

For Cu-TO

$Q_{theoretical} = (1x26.801\times10^3) / (3.6*470.5325) \text{ mA h g}^{-1}$

$Q_{theoretical} = 158.21908 \sim 158.2$

Electrochemical properties of full cell (Graphite (C_6)/Al, Ca, Cu-LTO cell)

Electrochemical properties of C_6/Al-LTO cell

The average voltage of Al-LTO with respect to Li metal is represented as

$V = -[E(\text{Al-LTO}) + E(C_6) - E(LiC_6) - E(\text{Al-L}_{1-x}\text{TO})]/F$---------- (1)

V=-[((-7699.051) + (-55.261eV) - (-260.303eV) - (-7488.592) eV]/(96.5 kJ/mol)

V= 5.417671692 V ~ 5.4 V

Oxidation potential of **C_6/Al-LTO** cell

$V_{ox}(\text{vs.}Li^+/C_6) = [E(\text{Al-LTO}) - E(\text{Al-L}_{1-x}\text{TO}) - E(\text{Li})]/F + E_{\circ\text{SCE /SHE}}(0.24) - E_{\circ(\text{Li+/C6})/\text{SHE}}(-3.0$ V)

$V_{ox}(\text{vs.}Li^+/C_6) = [(-7699.051) - (-7488.592) - (-204.706)] / (96.5\text{kJ/mol}) + 0.24 - 3.0 \text{ V}$

$V_{ox}(\text{vs.}Li^+/C_6) = 5.754069732 \text{ V} + 0.24 - 3.0 \text{ V} = 2.99 \text{ V}$

Reduction potential of **C_6/Al-LTO** cell is given as

V_{rox} (vs. Li^+/C_6) = [E (Al-LTO) – E (Al-L_{1-x}TO) – E (Li)]/$F - E_{\circ(Li+/C6)/SCE}$ ------- (8)

V_{rx}(vs.Li^+/C_6) = [(-7699.051) - (-7488.592) - (-204.706)] / (96.5kJ/mol) -3.0 V

V_{rx} (vs. Li^+/Li) = 5.754069732 V- 3.0 V = 2.75 V

Gravimetric energy density of **C_6/Al-LTO** cell

V = -[E(Al-LTO) + E(C_6) - E(LiC_6) - E(Al-L_{1-x}TO)]/m_{av} ----------(9) [1]

V=-[(-7699.051) + (-55.261) - (-260.303eV) - (-7488.5913eV)]/[2430.4335x10^{-24}/6.022 10^{-24} mol

V = [5.412 eV)]/[2430.4335 x 10^{-24}/6.022 10^{-24} mol

V = [5.412 x 96.485 kJ/mol)]/40.3592411 g/mol, [1eV = 4.45 Wh]

V = [3.99 x 96.485 kJ)]/40.3592411 g = 12.93822197 kJ/g

= 12.93822197 x 0.278 Wh/g = 3.596825708 Wh/g

= 3.60 kW h kg^{-1}

Gravimetrical energy density of **C_6/Al-LTO** cell = 3.60 kW h kg^{-1}

Gravimetrical power density of **C_6/Al-LTO** cell = 3.60 kW kg^{-1}

Electrochemical properties of Ca-LTO cell

Average voltage of **C_6**/Ca-LTO cell,

V= -[E(Ca-LTO) +E(C_6)-E(LiC_6)-E(Ca-L_{1-x}TO)]/F ---(6)[1]

V=-[(-15255.096) + (-55.261) - (-260.303) - (-15046.034) eV]/96.5kJ/mol

V= -[-4.02024165 eV)]/96.5kJ/mol

V= -[-4.02024165 eV eV)]/96.5kJ/mol = 4.02 V [1eV = 96.5kJ/mol]

Oxidation potential of **C_6**/Ca-LTO cell

V_{ox} (vs. Li^+/C_6) = [E (Ca-LTO) – E (Ca-L_{1-x}TO) – E (Li)]/F+ $E_{\circ\ SCE\ /SHE}$ (0.24)- $E_{\circ(Li+/C6)/SHE}$ (-3.0 V)

V_{ox} (vs. Li^+/C_6) = [(-15255.096) - (-15046.034) -(-204.706)]/ 96.5 kJ/mol + 0.24V-3.0 V

= 4.36 V + 0.24 V-3.0 V =1.6 V

Reduction potential of $\mathbf{C_6}$/Ca-LTO cell

V_{rx} (vs. Li^+/C_6) = [E(Ca-LTO) − E(Ca-L_{1-x}TO)]/F − $E_{\circ(Li^+/C6)/SCE}$ Eqn. S20

where M′ = Mn, Fe, Ni, F is Faraday's constant. $E_{(Li+/C6)/SCE}$ (-3.0 V) are the potentials of metallic lithium with respect to saturated calomel electrode

V_{ox} (vs. $Li+/C_6$) = [(-15255.096) - (-15046.034) - (-204.706)]/ 96.5 kJ/mol+0.24V-3.0 V

= 4.36 V-3.0 V =1.36 V

Gravimetric energy density of C_6/Ca-LTO cell is expressed as

γ = − [E (Ca-LTO) + E (C_6) – E (LiC_6) – E (Ca-L_{1-x}TO)]/m_{av} ----------(3)

γ = − [(-15255.096) + (-55.261) - (-260.303) - (-15046.0344)]/16.8073656 g/mol

γ = [4.02 x 96.485 x 2.77778 e-4 kW h/~~mol~~]/(16.8073656 g/~~mol~~)

γ = [2.324263595 kW h/kg] ~ 2.32 kW h/kg

Gravimetric energy density = 2.32 kW h/kg

Gravimetric power density = 2.32 kW/kg

Electrochemical properties of $\mathbf{C_6}$/Cu-LTO

The average voltage of Cu-LTO with respect to C_6 metal is represented as

V = − [E (Cu-LTO) + E (C_6) – E (LiC_6) – E (Cu-L_{1-x}TO)]/F ---------- (1)

V =-[(-35171.849) + (-55.261) - (-260.303) - (-34962.419)]/96.5 kJ/mol

V = [4.387950704 V] ~ 4.4 V

Oxidation potential of $\mathbf{C_6}$/Cu-LTO

V_{ox} (vs. $Li^+/\mathbf{C_6}$) = [E (Cu-LTO) – E (Cu-L_{1-x}TO) – E (Li)]/F+ $E_{SCE\ /SHE}$ − $E_{(Li+/\mathbf{C6})/SHE}$

V_{ox}(vs.Li^+/Li)=[(-35171.849) - (-34962.419) - (-204.706)]/96.5 kJ/mol+0.24-3.0 V

= 4.724931104 V + 0.24 V-3.0 V = 1.924931104 ~ 1.9 V

Reduction potential is given as

V_{rx} (vs. $Li^+/\mathbf{C_6}$) = [E (Cu-LTO) – E (Cu-L_{1-x}TO) – E (Li)]/F − $E_{\circ(Li+/Li)/SCE}$

V_{ox}(vs.Li^+/Li)=[(-35171.849)-(-34962.4193)-(-204.706)]/96.5kJ/mol-3.0 V

= 4.724931104 V-3.0 V = 1.724931 ~ 1.73 V

Gravimetric energy is expressed as

$\gamma = -[E(\text{Cu-LTO}) + E(C_6) - E(LiC_6) - E(\text{Cu-}L_{1-x}TO]/m_{av}$ ----------(3)

where m_{av} is the average mass of a fully relaxed ground state structure

$\gamma = -$ [(-35171.849) + (-55.261) - (-260.303) -(-34962.419)]/19.09597217g/mol

= [4.387950704 x 96.485 x 2.77778 e-4 kW h/~~mol~~]/ 19.09597217g/~~mol~~

= 6.158537869 kW h/kg

Gravimetric energy density = 6.158537869 kW h/kg ~ 6.2 kW h/kg

Gravimetric power density = ~ 6.2 kW/kg

Charge-discharge mechanism

Discussion about the effects of doping on the charge-discharge mechanism

- Al, Ca, Cu-doping into the 16d octahedral site of Ti induces excess electron into conduction band.
- The subsequent energy level provides channel for transmission of electrons from valance band (VB) to conduction band (CB) across the Fermi level and these energy levels tune the energy gap and improve the conductivity.
- Charge distribution analysis demonstrates the Li-ion diffusion along [101] direction and follow wave like pathways.
- Therefore, Multivalent metallic ion doping effectively improve high-rate discharge capacity, cyclic stability and lithium diffusion coefficient in LTO during charge-discharge processes.

- The chemical energy releases from Al-LTO due to dissociation of Li-ion, electron during de-intercalation (charging) and creates the structural dis-order (entropy) corresponding equation is given below

$$\text{Al (Ca, Cu)-LTO} \rightarrow \text{Al (Ca, Cu) -L}_{1-x}\text{TO} + \text{Li}^{+} + \text{e}^{-} + \Delta G$$

- ΔG, change in Gibbs free energy is given by

  For Li-ion de-intercalation (charging) in Al-LTO

  $\Delta G = G_{\text{Al-D-LTO}} - G_{\text{Al-LTO}} = -6558.02 - (-4160.25) = -2397.77$ J

  $\Delta G < 0$ strong adsorption, exothermic, spontaneous process

  The energy of -2397.77 J is useful for ejection of electron from cathode materials during charging

- For Li-ion de-intercalation in Ca-LTO

  $\Delta G = G_{\text{Ca-D-LTO}} - G_{\text{Ca-LTO}} = 21464.04 - (10775.1) = 10688.9$ J

  $\Delta G > 0$ weak adsorption, endothermic

- For Li-ion de-intercalation in Cu-LTO

  $\Delta G = G_{\text{Cu-D-LTO}} - G_{\text{Cu-LTO}} = -13242 - (-12939.08) = 303$ J

  $\Delta G < 0$ strong adsorption, exothermic

- The released energy utilized for Li^{+}-intercalation during discharge
  - $\text{Al (Ca, Cu) -L}_{1-x}\text{TO} + \text{Li}^{+} + \text{e}^{-} + \Delta G \rightarrow \text{Al (Ca, Cu)-LTO}$
- This process continues during cyclic performance.
- The volumetric and reversible change, internal strain and stress arises due to charge-discharge process that leads to development of micro cracks, shear and bulk anisotropy, capacity fading.
- Al, Ca, Cu-doping into LTO provides mechanical stability and superiority that offers strong ability to withstanding volumetric and reversible change, internal strain and

stress, against shear and bulk anisotropy which reduces micro cracks, capacity fading during Li-ion intercalation/de-intercalation was explained by mechanical properties.

- The chemical potential arises at positive/negative electrodes due to Li^+-intercalation/de-intercalation. The change in chemical potential is

$$\mu_{Al\text{-}LTO} - \mu_{Al\text{-}L(1\text{-}x)TO} = \Delta H_f$$

- Oxidation/reduction occur due to dissociation of Li^+ (Al, Ca, Cu), e^- under externally applied voltage and corresponding potential are called re-dox potential.
- Specific capacity increases from initial Al-LTO, Al-D-LTO compound (183.04, 189.47 mA h g^{-1}) to fully de-lithiated Al-TO compound (196.4 mA h g^{-1}) as compared undoped LTO (175 mA h g^{-1})
- The gravimetric energy and power densities and volumetric energy and power densities are increase through the doping of multivalent cations (Al, Ca, Cu).

```
OpenGL version: 4.6.14761 Compatibility Profile Context 21.30.44 30.0.13044.0
Video configuration: AMD Radeon(TM) Graphics
Maximum supported width and height of the viewport: 16384 x 16384
OpenGL depth buffer bit: 16


C:\simulation\Anod\Li4Ti5O12.cif
================================================================================
=
Title               Li4Ti5O12

Lattice type        F
Space group name    F d -3 m
Space group number  227
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 8.35700  8.35700  8.35700  90.0000  90.0000  90.0000

Unit-cell volume = 583.648349 Å^3

Structure parameters

                       x          y          z          Occ.     U    Site
Sym.
   1 Li  Li1         0.00000    0.00000    0.00000    1.000    0.000    8a      -
43m
   2 Li  Li2         0.62500    0.62500    0.62500    0.167    0.000   16d      .-
3m
```

```
   3 Ti  Ti1          0.62500    0.62500    0.62500    0.833    0.000   16d      .-
3m
   4 O   O1           0.38900    0.38900    0.38900    1.000    0.000   32e
.3m
================================================================================
=

Number of polygons and unique vertices on isosurface = 0 (0)
130 atoms, 168 bonds, 34 polyhedra; CPU time = 10 ms


POLYHEDRON:
   1     Li1 Li  0.50000  0.50000  1.00000  ( 0, 0, 1)+ -x+1/2, y+1/2, -z
--------------------------------------------------------------------------------
   4      O1  O  0.36100  0.36100  0.86100  ( 0, 0, 1)+ -y+3/4, -x+3/4, -z+1/4
   4      O1  O  0.36100  0.63900  1.13900  ( 0, 0, 0)+ -x+3/4, y+1/4, z+3/4
   4      O1  O  0.63900  0.36100  1.13900  ( 0, 0, 0)+ y+1/4, -x+3/4, z+3/4
   4      O1  O  0.63900  0.63900  0.86100  ( 0, 0, 1)+ x+1/4, y+1/4, -z+1/4
--------------------------------------------------------------------------------

l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
---------------------------------------
Average bond length =  2.0120 Å
Polyhedral volume =  4.1799 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation = 1.0000
Bond angle variance =  0.0000 deg.^2
Effective coordination number =  4.0000

Charge distribution
--------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
--------------------------------------------------------------------------------
                    x        y        z      delta_q    Q      q
   4      O1  O  0.36100  0.36100  0.86100    0.250 -2.000 -2.000
   4      O1  O  0.36100  0.63900  1.13900    0.250 -2.000 -2.000
   4      O1  O  0.63900  0.36100  1.13900    0.250 -2.000 -2.000
   4      O1  O  0.63900  0.63900  0.86100    0.250 -2.000 -2.000
--------------------------------------------------------------------------------
   1     Li1 Li  0.50000  0.50000  1.00000           1.000  1.000

Input a bond valence parameter: 0.370000
Bond valence of O1: -0.0118218
Bond valence of O1: -0.0118218
Bond valence of O1: -0.0118218
Bond valence of O1: -0.0118218
Bond valence sum = 0.047
Oxidation state of the cation: +1
Expected bond length = 0.883 Å

POLYHEDRON:
   2     Li2 Li  0.12500  0.37500  0.87500  (-1, 1, 1)+ x+1/2, -y, -z+1/2
--------------------------------------------------------------------------------
   4      O1  O -0.11100  0.38900  0.88900  (-1, 0, 0)+ x+1/2, y, z+1/2
   4      O1  O  0.11100  0.38900  1.11100  ( 0, 0, 1)+ -x+1/2, y, -z+1/2
   4      O1  O  0.11100  0.61100  0.88900  ( 0, 1, 0)+ -y+1/2, -x, z+1/2
   4      O1  O  0.13900  0.13900  0.86100  (-1,-1, 1)+ y+3/4, x+3/4, -z+1/4
   4      O1  O  0.13900  0.36100  0.63900  (-1, 0, 0)+ x+3/4, -y+3/4, z+1/4
   4      O1  O  0.36100  0.36100  0.86100  ( 0, 0, 1)+ -y+3/4, -x+3/4, -z+1/4
--------------------------------------------------------------------------------

l(Li2-O1) =  1.97918(0) Å
l(Li2-O1) =  1.97918(0) Å
```

```
l(Li2-O1) =  1.97918(0) Å
l(Li2-O1) =  1.97918(0) Å
l(Li2-O1) =  1.97918(0) Å
l(Li2-O1) =  1.97918(0) Å
---------------------------------------
Average bond length =  1.9792 Å
Polyhedral volume = 10.1251 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0139
Bond angle variance =  52.9620 deg.^2
Effective coordination number =  6.0000

Charge distribution
-------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
-------------------------------------------------------------------------------
                   x        y        z      delta_q    Q      q
   4      O1  O -0.11100  0.38900  0.88900    0.583 -2.000 -2.000
   4      O1  O  0.11100  0.38900  1.11100    0.583 -2.000 -2.000
   4      O1  O  0.11100  0.61100  0.88900    0.583 -2.000 -2.000
   4      O1  O  0.13900  0.13900  0.86100    0.583 -2.000 -2.000
   4      O1  O  0.13900  0.36100  0.63900    0.583 -2.000 -2.000
   4      O1  O  0.36100  0.36100  0.86100    0.583 -2.000 -2.000
-------------------------------------------------------------------------------
   2     Li2 Li  0.12500  0.37500  0.87500           3.500  3.500

Input a bond valence parameter: 0.370000
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence sum = 0.013
Oxidation state of the cation: +1
Expected bond length = 1.033 Å

130 atoms, 168 bonds, 34 polyhedra; CPU time = 9 ms

================================================================================
=
Title               Li4Ti5O12

Lattice type        F
Space group name    F d -3 m
Space group number  227
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 8.35700  8.35700  8.35700  90.0000  90.0000  90.0000

Unit-cell volume = 583.648349 Å^3

Structure parameters

                      x          y          z          Occ.     U    Site
Sym.
   1 Li  Li1         0.00000    0.00000    0.00000    1.000    0.000    8a      -
43m
   2 Li  Li2         0.62500    0.62500    0.62500    0.167    0.000   16d      .-
3m
   3 Ti  Ti1         0.62500    0.62500    0.62500    1.000    0.000   16d      .-
3m
```

```
   4 O   O1          0.38900    0.38900    0.38900    1.000    0.000   32e
.3m
================================================================================
=

Number of polygons and unique vertices on isosurface = 0 (0)
130 atoms, 168 bonds, 34 polyhedra; CPU time = 9 ms

106 atoms, 72 bonds, 18 polyhedra; CPU time = 5 ms

================================================================================
=
Title               Li1.333 O4 Ti1.667

Lattice type        F
Space group name    F d -3 m
Space group number  227
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 8.35700  8.35700  8.35700  90.0000  90.0000  90.0000

Unit-cell volume = 583.648349 Å^3

Structure parameters

                       x          y          z          Occ.     U    Site
Sym.
   1 Li  Li1         0.00000    0.00000    0.00000    1.000    0.000    8a      -
43m
   2 Ti  Ti1         0.62500    0.62500    0.62500    1.000    0.000   16d      .-
3m
   3 O   O1          0.38900    0.38900    0.38900    1.000    0.000   32e
.3m
================================================================================
=

Number of polygons and unique vertices on isosurface = 0 (0)
106 atoms, 72 bonds, 18 polyhedra; CPU time = 5 ms

130 atoms, 168 bonds, 34 polyhedra; CPU time = 9 ms

================================================================================
=
Title               Li4Ti5O12

Lattice type        F
Space group name    F d -3 m
Space group number  227
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 8.35700  8.35700  8.35700  90.0000  90.0000  90.0000

Unit-cell volume = 583.648349 Å^3

Structure parameters

                       x          y          z          Occ.     U    Site
Sym.
   1 Li  Li1         0.00000    0.00000    0.00000    1.000    0.000    8a      -
43m
   2 Li  Li2         0.62500    0.62500    0.62500    0.000    0.000   16d      .-
3m
```

```
   3 Ti  Ti1          0.62500    0.62500    0.62500    1.000    0.000   16d      .-
3m
   4 O   O1           0.38900    0.38900    0.38900    1.000    0.000   32e
.3m
================================================================================
=

Number of polygons and unique vertices on isosurface = 0 (0)
130 atoms, 168 bonds, 34 polyhedra; CPU time = 9 ms


POLYHEDRON:
   2     Li2 Li  0.62500  0.87500  0.87500  ( 1, 0, 0)+ -x+1/4, y+1/4, z+1/4
--------------------------------------------------------------------------------
   4      O1  O  0.38900  0.88900  0.88900  ( 0, 0, 0)+ x, y+1/2, z+1/2
   4      O1  O  0.63900  0.63900  0.86100  ( 0, 0, 1)+ x+1/4, y+1/4, -z+1/4
   4      O1  O  0.63900  0.86100  0.63900  ( 0, 1, 0)+ y+1/4, -x+1/4, z+1/4
   4      O1  O  0.61100  0.88900  1.11100  ( 1, 0, 1)+ -y, x+1/2, -z+1/2
   4      O1  O  0.61100  1.11100  0.88900  ( 1, 1, 0)+ -x, -y+1/2, z+1/2
   4      O1  O  0.86100  0.86100  0.86100  ( 1, 1, 1)+ -y+1/4, -x+1/4, -z+1/4
--------------------------------------------------------------------------------

l(Li2-O1) =  1.97918(0) Å
l(Li2-O1) =  1.97918(0) Å
l(Li2-O1) =  1.97918(0) Å
l(Li2-O1) =  1.97918(0) Å
l(Li2-O1) =  1.97918(0) Å
l(Li2-O1) =  1.97918(0) Å
---------------------------------------
Average bond length =  1.9792 Å
Polyhedral volume = 10.1251 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0139
Bond angle variance =  52.9620 deg.^2
Effective coordination number =  6.0000

Charge distribution
--------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
--------------------------------------------------------------------------------
                    x        y        z      delta_q    Q      q
   4      O1  O  0.38900  0.88900  0.88900    0.667 -2.250 -2.000
   4      O1  O  0.63900  0.63900  0.86100    0.667 -2.250 -2.000
   4      O1  O  0.63900  0.86100  0.63900    0.667 -2.250 -2.000
   4      O1  O  0.61100  0.88900  1.11100    0.667 -2.250 -2.000
   4      O1  O  0.61100  1.11100  0.88900    0.667 -2.250 -2.000
   4      O1  O  0.86100  0.86100  0.86100    0.667 -2.250 -2.000
--------------------------------------------------------------------------------
   2     Li2 Li  0.62500  0.87500  0.87500           3.556  4.000

Input a bond valence parameter: 0.370000
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence sum = 0.000
Oxidation state of the cation: +1
Expected bond length = 1.033 Å
106 atoms, 72 bonds, 18 polyhedra; CPU time = 6 ms

================================================================================
=
Title               Li1.333 O4 Ti1.667
```

```
Lattice type        F
Space group name    F d -3 m
Space group number  227
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 8.35700  8.35700  8.35700  90.0000  90.0000  90.0000

Unit-cell volume = 583.648349 Å^3

Structure parameters

                       x          y          z          Occ.     U    Site
Sym.
   1 Li  Li1         0.00000    0.00000    0.00000    1.000    0.000    8a      -
43m
   2 Ti  Ti2         0.62500    0.62500    0.62500    0.167    0.000   16d      .-
3m
   3 Ti  Ti1         0.62500    0.62500    0.62500    1.000    0.000   16d      .-
3m
   4 O   O1          0.38900    0.38900    0.38900    1.000    0.000   32e
.3m
================================================================================
=

Number of polygons and unique vertices on isosurface = 0 (0)
106 atoms, 72 bonds, 18 polyhedra; CPU time = 6 ms

Atom:  2   Ti2  Ti   0.62500   0.87500   0.87500  ( 1, 0, 0)+ -x+1/4, y+1/4, z+1/4
          (x,y,z):   5.22313   7.31238   7.31238
              Occ. = 0.167         Ueq = 0.00000     16d    .-3m
106 atoms, 72 bonds, 18 polyhedra; CPU time = 6 ms

================================================================================
=
Title               Li1.333 O4 Ti1.667

Lattice type        F
Space group name    F d -3 m
Space group number  227
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 8.35700  8.35700  8.35700  90.0000  90.0000  90.0000

Unit-cell volume = 583.648349 Å^3

Structure parameters

                       x          y          z          Occ.     U    Site
Sym.
   1 Li  Li1         0.00000    0.00000    0.00000    1.000    0.000    8a      -
43m
   2 Ti  Ti2         0.62500    0.62500    0.62500    0.167    0.000   16d      .-
3m
   3 Ti  Ti1         0.62500    0.62500    0.62500    1.000    0.000   16d      .-
3m
   4 O   O1          0.38900    0.38900    0.38900    1.000    0.000   32e
.3m
================================================================================
=

Number of polygons and unique vertices on isosurface = 0 (0)
106 atoms, 72 bonds, 18 polyhedra; CPU time = 6 ms
```

```
130 atoms, 168 bonds, 34 polyhedra; CPU time = 10 ms

130 atoms, 168 bonds, 34 polyhedra; CPU time = 9 ms


POLYHEDRON:
   2     Ti2 Ti  0.12500  0.37500  0.87500  (-1, 1, 1)+ x+1/2, -y, -z+1/2
-------------------------------------------------------------------------------
   4      O1  O -0.11100  0.38900  0.88900  (-1, 0, 0)+ x+1/2, y, z+1/2
   4      O1  O  0.11100  0.38900  1.11100  ( 0, 0, 1)+ -x+1/2, y, -z+1/2
   4      O1  O  0.11100  0.61100  0.88900  ( 0, 1, 0)+ -y+1/2, -x, z+1/2
   4      O1  O  0.13900  0.13900  0.86100  (-1,-1, 1)+ y+3/4, x+3/4, -z+1/4
   4      O1  O  0.13900  0.36100  0.63900  (-1, 0, 0)+ x+3/4, -y+3/4, z+1/4
   4      O1  O  0.36100  0.36100  0.86100  ( 0, 0, 1)+ -y+3/4, -x+3/4, -z+1/4
-------------------------------------------------------------------------------

l(Ti2-O1) =  1.97918(0) Å
l(Ti2-O1) =  1.97918(0) Å
l(Ti2-O1) =  1.97918(0) Å
l(Ti2-O1) =  1.97918(0) Å
l(Ti2-O1) =  1.97918(0) Å
l(Ti2-O1) =  1.97918(0) Å
--------------------------------------
Average bond length =  1.9792 Å
Polyhedral volume = 10.1251 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0139
Bond angle variance =  52.9620 deg.^2
Effective coordination number =  6.0000

Charge distribution
-------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
-------------------------------------------------------------------------------
                  x        y        z      delta_q    Q      q
   4      O1  O -0.11100  0.38900  0.88900    0.778 -2.583 -2.000
   4      O1  O  0.11100  0.38900  1.11100    0.778 -2.583 -2.000
   4      O1  O  0.11100  0.61100  0.88900    0.778 -2.583 -2.000
   4      O1  O  0.13900  0.13900  0.86100    0.778 -2.583 -2.000
   4      O1  O  0.13900  0.36100  0.63900    0.778 -2.583 -2.000
   4      O1  O  0.36100  0.36100  0.86100    0.778 -2.583 -2.000
-------------------------------------------------------------------------------
   2     Ti2 Ti  0.12500  0.37500  0.87500           3.613  4.667

Input a bond valence parameter: 0.370000
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence sum = 0.013
Oxidation state of the cation: +4
Expected bond length = 0.520 Å


OpenGL version: 4.6.14761 Compatibility Profile Context 21.30.44 30.0.13044.0
Video configuration: AMD Radeon(TM) Graphics
Maximum supported width and height of the viewport: 16384 x 16384
OpenGL depth buffer bit: 16


C:\Users\kiran kumar\Desktop\ Li4 O12 Ti2.5Al2.5.cif
================================================================================
=
```

```
================================================================================
=
Title               Li4 O12 Ti2.5Al2.5

Lattice type        F
Space group name    F d -3 m
Space group number  227
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 8.35700  8.35700  8.35700  90.0000  90.0000  90.0000

Unit-cell volume = 583.648349 Å^3

Structure parameters

                       x          y          z          Occ.     U    Site
Sym.
   1 Li  Li1          0.00000    0.00000    0.00000    1.000    0.000    8a      -
43m
   2 Al  Al2          0.62500    0.62500    0.62500    0.500    0.000   16d      .-
3m
   3 Ti  Ti1          0.62500    0.62500    0.62500    0.500    0.000   16d      .-
3m
   4 O   O1           0.38900    0.38900    0.38900    1.000    0.000   32e
.3m
================================================================================
=

Number of polygons and unique vertices on isosurface = 0 (0)
106 atoms, 72 bonds, 18 polyhedra; CPU time = 4 ms

130 atoms, 168 bonds, 34 polyhedra; CPU time = 7 ms

130 atoms, 168 bonds, 34 polyhedra; CPU time = 7 ms

130 atoms, 168 bonds, 34 polyhedra; CPU time = 6 ms

130 atoms, 168 bonds, 34 polyhedra; CPU time = 6 ms

130 atoms, 168 bonds, 34 polyhedra; CPU time = 7 ms

130 atoms, 168 bonds, 34 polyhedra; CPU time = 7 ms

================================================================================
=
Title               Li4 O12 Ti2.5Al2.5

Lattice type        F
Space group name    F d -3 m
Space group number  227
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 8.35700  8.35700  8.35700  90.0000  90.0000  90.0000

Unit-cell volume = 583.648349 Å^3

Structure parameters

                       x          y          z          Occ.     U    Site
Sym.
   1 Li  Li1          0.00000    0.00000    0.00000    1.000    0.000    8a      -
43m
```

```
   2 Al  Al2          0.62500    0.62500    0.62500    0.500    0.000   16d      .-
3m
   3 Ti  Ti1          0.62500    0.62500    0.62500    0.500    0.000   16d      .-
3m
   4 O   O1           0.38900    0.38900    0.38900    1.000    0.000   32e
.3m
================================================================================
=

Number of polygons and unique vertices on isosurface = 0 (0)
130 atoms, 168 bonds, 34 polyhedra; CPU time = 7 ms


POLYHEDRON:
   1     Li1 Li  1.00000  0.50000  0.50000  ( 1, 0, 0)+ -x, -y+1/2, z+1/2
--------------------------------------------------------------------------
   4      O1  O  0.86100  0.36100  0.36100  ( 1, 0, 0)+ -y+1/4, -x+3/4, -z+3/4
   4      O1  O  0.86100  0.63900  0.63900  ( 1, 0, 0)+ -x+1/4, y+1/4, z+1/4
   4      O1  O  1.13900  0.36100  0.63900  ( 0, 0, 0)+ x+3/4, -y+3/4, z+1/4
   4      O1  O  1.13900  0.63900  0.36100  ( 0, 0, 0)+ y+3/4, x+1/4, -z+3/4
--------------------------------------------------------------------------

l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
---------------------------------------
Average bond length =  2.02 Å
Polyhedral volume =  4.18 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation = 1.0000
Bond angle variance =   0.0000 deg.^2
Effective coordination number =  4.0000

Charge distribution
--------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
--------------------------------------------------------------------------------
                    x        y        z      delta_q    Q      q
   4      O1  O  0.86100  0.36100  0.36100    0.253 -2.000 -2.000
   4      O1  O  0.86100  0.63900  0.63900    0.253 -2.000 -2.000
   4      O1  O  1.13900  0.36100  0.63900    0.253 -2.000 -2.000
   4      O1  O  1.13900  0.63900  0.36100    0.253 -2.000 -2.000
--------------------------------------------------------------------------
   1     Li1 Li  1.00000  0.50000  0.50000           1.000  1.000

Input a bond valence parameter: 0.370000
Bond valence of O1: -0.0118218
Bond valence of O1: -0.0118218
Bond valence of O1: -0.0118218
Bond valence of O1: -0.0118218
Bond valence sum = 0.049
Oxidation state of the cation: +1
Expected bond length = 0.883 Å

POLYHEDRON:
   1     Li2 Li  0.75000  0.25000  0.75000  ( 0, 0, 0)+ y+3/4, x+1/4, -z+3/4
--------------------------------------------------------------------------
   4      O1  O  0.61100  0.11100  0.88900  ( 1, 0, 0)+ -x, -y+1/2, z+1/2
   4      O1  O  0.61100  0.38900  0.61100  ( 1, 0, 1)+ -y, x, -z
   4      O1  O  0.88900  0.11100  0.61100  ( 0, 0, 1)+ y+1/2, -x+1/2, -z
   4      O1  O  0.88900  0.38900  0.88900  ( 0, 0, 0)+ x+1/2, y, z+1/2
--------------------------------------------------------------------------

l(Li2-O1) =  2.01199(0) Å
l(Li2-O1) =  2.01199(0) Å
```

```
l(Li2-O1) =  2.01199(0) Å
l(Li2-O1) =  2.01199(0) Å
---------------------------------------
Average bond length =  2.03 Å
Polyhedral volume =  4.199 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0000
Bond angle variance =   0.0000 deg.^2
Effective coordination number =  4.0000

Charge distribution
-------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
-------------------------------------------------------------------------------
                   x        y        z      delta_q    Q      q
   4      O1  O  0.61100  0.11100  0.88900    0.254 -2.000 -2.000
   4      O1  O  0.61100  0.38900  0.61100    0.254 -2.000 -2.000
   4      O1  O  0.88900  0.11100  0.61100    0.254 -2.000 -2.000
   4      O1  O  0.88900  0.38900  0.88900    0.254 -2.000 -2.000
-------------------------------------------------------------------------------
   1     Li2 Li  0.75000  0.25000  0.75000           1.000  1.000

Input a bond valence parameter: 0.370000
Bond valence of O1: -0.0118218
Bond valence of O1: -0.0118218
Bond valence of O1: -0.0118218
Bond valence of O1: -0.0118218
Bond valence sum = 0.05
Oxidation state of the cation: +1
Expected bond length = 0.883 Å
Atom:  4    O1   O   0.86100   1.13900   1.13900  ( 1, 0, 0)+ -y+1/4, x+3/4, z+3/4
          (x,y,z):   7.19538   9.51862   9.51862
              Occ. = 1.000         Ueq = 0.00000     32e     .3m




POLYHEDRON:
   2     Al1 Al  0.12500  0.37500  0.87500  (-1, 1, 1)+ x+1/2, -y, -z+1/2
-------------------------------------------------------------------------------
   4      O1  O -0.11100  0.38900  0.88900  (-1, 0, 0)+ x+1/2, y, z+1/2
   4      O1  O  0.11100  0.38900  1.11100  ( 0, 0, 1)+ -x+1/2, y, -z+1/2
   4      O1  O  0.11100  0.61100  0.88900  ( 0, 1, 0)+ -y+1/2, -x, z+1/2
   4      O1  O  0.13900  0.13900  0.86100  (-1,-1, 1)+ y+3/4, x+3/4, -z+1/4
   4      O1  O  0.13900  0.36100  0.63900  (-1, 0, 0)+ x+3/4, -y+3/4, z+1/4
   4      O1  O  0.36100  0.36100  0.86100  ( 0, 0, 1)+ -y+3/4, -x+3/4, -z+1/4
-------------------------------------------------------------------------------

l(Al1-O1) =  1.97918(0) Å
l(Al1-O1) =  1.97918(0) Å
l(Al1-O1) =  1.97918(0) Å
l(Al1-O1) =  1.97918(0) Å
l(Al1-O1) =  1.97918(0) Å
l(Al1-O1) =  1.97918(0) Å
---------------------------------------
Average bond length =  1.9792 Å
Polyhedral volume = 10.1251 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0139
Bond angle variance =  52.9620 deg.^2
Effective coordination number =  6.0000
```

```
Charge distribution
-------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
-------------------------------------------------------------------------------
                    x        y        z      delta_q    Q      q
   4      O1  O -0.11100  0.38900  0.88900    0.583 -2.000 -2.000
   4      O1  O  0.11100  0.38900  1.11100    0.583 -2.000 -2.000
   4      O1  O  0.11100  0.61100  0.88900    0.583 -2.000 -2.000
   4      O1  O  0.13900  0.13900  0.86100    0.583 -2.000 -2.000
   4      O1  O  0.13900  0.36100  0.63900    0.583 -2.000 -2.000
   4      O1  O  0.36100  0.36100  0.86100    0.583 -2.000 -2.000
-------------------------------------------------------------------------------
   2     Al1 Al  0.12500  0.37500  0.87500           3.500  3.500

Input a bond valence parameter: 0.370000
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence sum = 0.039
Oxidation state of the cation: +3
Expected bond length = 0.626 Å


================================================================================
=
Title               Li4 O12 Ti2.5Al2.5

Lattice type        F
Space group name    F d -3 m
Space group number  227
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 8.35700  8.35700  8.35700  90.0000  90.0000  90.0000

Unit-cell volume = 583.648349 Å^3

Structure parameters

                      x          y          z          Occ.     U    Site
Sym.
   1 Li  Li1         0.00000    0.00000    0.00000    1.000    0.000    8a      -
43m
   2 Al  Al1         0.62500    0.62500    0.62500    0.500    0.000   16d      .-
3m
   3 Ti  Ti1         0.62500    0.62500    0.62500    0.500    0.000   16d      .-
3m
   4 O   O1          0.38900    0.38900    0.38900    1.000    0.000   32e
.3m
================================================================================
=
Number of polygons and unique vertices on isosurface = 0 (0)
130 atoms, 168 bonds, 34 polyhedra; CPU time = 7 ms
POLYHEDRON:
   2     Ti1 Ti  0.87500  0.87500  0.62500  ( 0, 0, 1)+ x+1/4, y+1/4, -z+1/4
-------------------------------------------------------------------------------
   4      O1  O  0.63900  0.86100  0.63900  ( 0, 1, 0)+ y+1/4, -x+1/4, z+1/4
   4      O1  O  0.86100  0.63900  0.63900  ( 1, 0, 0)+ -x+1/4, y+1/4, z+1/4
   4      O1  O  0.86100  0.86100  0.86100  ( 1, 1, 1)+ -y+1/4, -x+1/4, -z+1/4
   4      O1  O  0.88900  0.88900  0.38900  ( 0, 0, 0)+ x+1/2, y+1/2, z
   4      O1  O  0.88900  1.11100  0.61100  ( 0, 1, 1)+ y+1/2, -x+1/2, -z
```

```
   4      O1  O  1.11100  0.88900  0.61100  ( 1, 0, 1)+ -x+1/2, y+1/2, -z
--------------------------------------------------------------------------------
l(Ti1-O1) =  1.97918(0) Å
l(Ti1-O1) =  1.97918(0) Å
l(Ti1-O1) =  1.97918(0) Å
l(Ti1-O1) =  1.97918(0) Å
l(Ti1-O1) =  1.97918(0) Å
l(Ti1-O1) =  1.97918(0) Å
---------------------------------------
Average bond length =  1.9792 Å
Polyhedral volume = 10.1251 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0139
Bond angle variance =  52.9620 deg.^2
Effective coordination number =  6.0000
Charge distribution
--------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
--------------------------------------------------------------------------------
                    x        y        z      delta_q    Q      q
   4      O1  O  0.63900  0.86100  0.63900    0.500 -1.750 -2.000
   4      O1  O  0.86100  0.63900  0.63900    0.500 -1.750 -2.000
   4      O1  O  0.86100  0.86100  0.86100    0.500 -1.750 -2.000
   4      O1  O  0.88900  0.88900  0.38900    0.500 -1.750 -2.000
   4      O1  O  0.88900  1.11100  0.61100    0.500 -1.750 -2.000
   4      O1  O  1.11100  0.88900  0.61100    0.500 -1.750 -2.000
--------------------------------------------------------------------------------
   2     Ti1 Ti  0.87500  0.87500  0.62500           3.429  3.000

Input a bond valence parameter: 0.370000
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence sum = 0.039
Oxidation state of the cation: +2
Expected bond length = 0.776 Å

OpenGL version: 4.6.14761 Compatibility Profile Context 21.30.44 30.0.13044.0
Video configuration: AMD Radeon(TM) Graphics
Maximum supported width and height of the viewport: 16384 x 16384
OpenGL depth buffer bit: 16

C:\Users\kiran kumar\Desktop\Li4Ti2.5Ca2.5O12.vesta
================================================================================
=
Title               Li4Ti2.5Ca2.5O12

Lattice type        F
Space group name    F d -3 m
Space group number  227
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 8.35700  8.35700  8.35700  90.0000  90.0000  90.0000

Unit-cell volume = 583.648349 Å^3

Structure parameters

                        x          y          z          Occ.     U    Site
Sym.
```

```
   1 Li  Li1          0.00000    0.00000    0.00000    1.000    0.000    8a      -
43m
   2 Ti  Ti2          0.62500    0.62500    0.62500    0.500    0.000   16d      .-
3m
   3 Ca  Ca1          0.62500    0.62500    0.62500    0.500    0.000   16d      .-
3m
   4 O   O1           0.38900    0.38900    0.38900    1.000    0.000   32e
.3m
================================================================================
=

Number of polygons and unique vertices on isosurface = 0 (0)
130 atoms, 168 bonds, 34 polyhedra; CPU time = 24 ms

POLYHEDRON:
   2     Ti2 Ti  0.62500  0.87500  0.87500  ( 1, 0, 0)+ -x+1/4, y+1/4, z+1/4
--------------------------------------------------------------------------------
   4      O1  O  0.38900  0.88900  0.88900  ( 0, 0, 0)+ x, y+1/2, z+1/2
   4      O1  O  0.63900  0.63900  0.86100  ( 0, 0, 1)+ x+1/4, y+1/4, -z+1/4
   4      O1  O  0.63900  0.86100  0.63900  ( 0, 1, 0)+ y+1/4, -x+1/4, z+1/4
   4      O1  O  0.61100  0.88900  1.11100  ( 1, 0, 1)+ -y, x+1/2, -z+1/2
   4      O1  O  0.61100  1.11100  0.88900  ( 1, 1, 0)+ -x, -y+1/2, z+1/2
   4      O1  O  0.86100  0.86100  0.86100  ( 1, 1, 1)+ -y+1/4, -x+1/4, -z+1/4
--------------------------------------------------------------------------------
l(Ti2-O1) =  1.97918(0) Å
l(Ti2-O1) =  1.97918(0) Å
l(Ti2-O1) =  1.97918(0) Å
l(Ti2-O1) =  1.97918(0) Å
l(Ti2-O1) =  1.97918(0) Å
l(Ti2-O1) =  1.97918(0) Å
----------------------------------------
Average bond length =  1.98 Å
Polyhedral volume = 10.1251 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0139
Bond angle variance =  52.97 deg.^2
Effective coordination number =  6.0000

Input a bond valence parameter: 0.370000
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence sum = 0.039
Oxidation state of the cation: +4
Expected bond length = 0.520 Å
106 atoms, 72 bonds, 18 polyhedra; CPU time = 6 ms

================================================================================
=
Title               Li4Ti2.5Ca2.5O12

Lattice type        F
Space group name    F d -3 m
Space group number  227
Setting number      1
Lattice parameters
  a        b        c       alpha    beta     gamma
 8.35700  8.35700  8.35700  90.0000  90.0000  90.0000

Unit-cell volume = 583.648349 Å^3

Structure parameters
                       x          y          z          Occ.     U    Site
Sym.
```

```
   1 Li  Li1          0.00000    0.00000    0.00000    1.000    0.000    8a      -
43m
   2 Ca  Ca2          0.62500    0.62500    0.62500    0.500    0.000   16d      .-
3m
   3 Ca  Ca1          0.62500    0.62500    0.62500    0.500    0.000   16d      .-
3m
   4 O   O1           0.38900    0.38900    0.38900    1.000    0.000   32e
.3m
================================================================================
=

Number of polygons and unique vertices on isosurface = 0 (0)
106 atoms, 72 bonds, 18 polyhedra; CPU time = 6 ms
106 atoms, 72 bonds, 18 polyhedra; CPU time = 6 ms
130 atoms, 168 bonds, 34 polyhedra; CPU time = 9 ms
130 atoms, 168 bonds, 34 polyhedra; CPU time = 9 ms
POLYHEDRON:
   2     Ca2 Ca  0.12500  0.37500  0.87500  (-1, 1, 1)+ x+1/2, -y, -z+1/2
--------------------------------------------------------------------------------
   4      O1  O -0.11100  0.38900  0.88900  (-1, 0, 0)+ x+1/2, y, z+1/2
   4      O1  O  0.11100  0.38900  1.11100  ( 0, 0, 1)+ -x+1/2, y, -z+1/2
   4      O1  O  0.11100  0.61100  0.88900  ( 0, 1, 0)+ -y+1/2, -x, z+1/2
   4      O1  O  0.13900  0.13900  0.86100  (-1,-1, 1)+ y+3/4, x+3/4, -z+1/4
   4      O1  O  0.13900  0.36100  0.63900  (-1, 0, 0)+ x+3/4, -y+3/4, z+1/4
   4      O1  O  0.36100  0.36100  0.86100  ( 0, 0, 1)+ -y+3/4, -x+3/4, -z+1/4
--------------------------------------------------------------------------------
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
---------------------------------------
Average bond length =  1.982 Å
Polyhedral volume = 10.126 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0143
Bond angle variance =  52.974 deg.^2
Effective coordination number =  6.0000
Input a bond valence parameter: 0.370000
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence sum = 0.039
Oxidation state of the cation: +2
Expected bond length = 0.776 Å
POLYHEDRON:
   2     Ca2 Ca  0.62500  0.87500  0.87500  ( 1, 0, 0)+ -x+1/4, y+1/4, z+1/4
--------------------------------------------------------------------------------
   4      O1  O  0.38900  0.88900  0.88900  ( 0, 0, 0)+ x, y+1/2, z+1/2
   4      O1  O  0.63900  0.63900  0.86100  ( 0, 0, 1)+ x+1/4, y+1/4, -z+1/4
   4      O1  O  0.63900  0.86100  0.63900  ( 0, 1, 0)+ y+1/4, -x+1/4, z+1/4
   4      O1  O  0.61100  0.88900  1.11100  ( 1, 0, 1)+ -y, x+1/2, -z+1/2
   4      O1  O  0.61100  1.11100  0.88900  ( 1, 1, 0)+ -x, -y+1/2, z+1/2
   4      O1  O  0.86100  0.86100  0.86100  ( 1, 1, 1)+ -y+1/4, -x+1/4, -z+1/4
--------------------------------------------------------------------------------

l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
---------------------------------------
Average bond length =  1.9792 Å
```

```
Polyhedral volume = 10.1251 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0139
Bond angle variance =  52.9620 deg.^2
Effective coordination number =  6.0000
Input a bond valence parameter: 1.000000
Bond valence of O1: -0.0709036
Bond valence of O1: -0.0709036
Bond valence of O1: -0.0709036
Bond valence of O1: -0.0709036
Bond valence of O1: -0.0709036
Bond valence of O1: -0.0709036
Bond valence sum = 0.213
Oxidation state of the cation: +2
Expected bond length = 1.406 Å

POLYHEDRON:
   1     Li1 Li  0.50000  0.50000  1.00000  ( 0, 0, 1)+ -x+1/2, y+1/2, -z
--------------------------------------------------------------------------
   4      O1  O  0.36100  0.36100  0.86100  ( 0, 0, 1)+ -y+3/4, -x+3/4, -z+1/4
   4      O1  O  0.36100  0.63900  1.13900  ( 0, 0, 0)+ -x+3/4, y+1/4, z+3/4
   4      O1  O  0.63900  0.36100  1.13900  ( 0, 0, 0)+ y+1/4, -x+3/4, z+3/4
   4      O1  O  0.63900  0.63900  0.86100  ( 0, 0, 1)+ x+1/4, y+1/4, -z+1/4
--------------------------------------------------------------------------

l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
---------------------------------------
Average bond length =  2.0120 Å
Polyhedral volume =  4.1799 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0000
Bond angle variance =   0.0000 deg.^2
Effective coordination number =  4.0000


POLYHEDRON:
   1     Li1 Li  0.50000  0.50000  1.00000  ( 0, 0, 1)+ -x+1/2, y+1/2, -z
--------------------------------------------------------------------------
   4      O1  O  0.36100  0.36100  0.86100  ( 0, 0, 1)+ -y+3/4, -x+3/4, -z+1/4
   4      O1  O  0.36100  0.63900  1.13900  ( 0, 0, 0)+ -x+3/4, y+1/4, z+3/4
   4      O1  O  0.63900  0.36100  1.13900  ( 0, 0, 0)+ y+1/4, -x+3/4, z+3/4
   4      O1  O  0.63900  0.63900  0.86100  ( 0, 0, 1)+ x+1/4, y+1/4, -z+1/4
--------------------------------------------------------------------------

l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
---------------------------------------
Average bond length =  2.0120 Å
Polyhedral volume =  4.1799 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0000
Bond angle variance =   0.0000 deg.^2
Effective coordination number =  4.0000

Input a bond valence parameter: 1.000000
Bond valence of O1: -0.064887
Bond valence of O1: -0.064887
Bond valence of O1: -0.064887
Bond valence of O1: -0.064887
Bond valence sum = 0.260
Oxidation state of the cation: +1
Expected bond length = 1.513 Å
```

```
POLYHEDRON:
   2     Ca2 Ca  0.12500  0.37500  0.87500  (-1, 1, 1)+ x+1/2, -y, -z+1/2
-------------------------------------------------------------------------------
   4      O1  O -0.11100  0.38900  0.88900  (-1, 0, 0)+ x+1/2, y, z+1/2
   4      O1  O  0.11100  0.38900  1.11100  ( 0, 0, 1)+ -x+1/2, y, -z+1/2
   4      O1  O  0.11100  0.61100  0.88900  ( 0, 1, 0)+ -y+1/2, -x, z+1/2
   4      O1  O  0.13900  0.13900  0.86100  (-1,-1, 1)+ y+3/4, x+3/4, -z+1/4
   4      O1  O  0.13900  0.36100  0.63900  (-1, 0, 0)+ x+3/4, -y+3/4, z+1/4
   4      O1  O  0.36100  0.36100  0.86100  ( 0, 0, 1)+ -y+3/4, -x+3/4, -z+1/4
-------------------------------------------------------------------------------

l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
---------------------------------------
Average bond length =  1.9792 Å
Polyhedral volume = 10.1251 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0139
Bond angle variance =  52.9620 deg.^2
Effective coordination number =  6.0000

POLYHEDRON:
   2     Ca2 Ca  0.62500  0.87500  0.87500  ( 1, 0, 0)+ -x+1/4, y+1/4, z+1/4
-------------------------------------------------------------------------------
   4      O1  O  0.38900  0.88900  0.88900  ( 0, 0, 0)+ x, y+1/2, z+1/2
   4      O1  O  0.63900  0.63900  0.86100  ( 0, 0, 1)+ x+1/4, y+1/4, -z+1/4
   4      O1  O  0.63900  0.86100  0.63900  ( 0, 1, 0)+ y+1/4, -x+1/4, z+1/4
   4      O1  O  0.61100  0.88900  1.11100  ( 1, 0, 1)+ -y, x+1/2, -z+1/2
   4      O1  O  0.61100  1.11100  0.88900  ( 1, 1, 0)+ -x, -y+1/2, z+1/2
   4      O1  O  0.86100  0.86100  0.86100  ( 1, 1, 1)+ -y+1/4, -x+1/4, -z+1/4
-------------------------------------------------------------------------------

l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
---------------------------------------
Average bond length =  1.9792 Å
Polyhedral volume = 10.1251 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0139
Bond angle variance =  52.9620 deg.^2
Effective coordination number =  6.0000

Input a bond valence parameter: 0.370000
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence sum = 0.039
Oxidation state of the cation: +2
Expected bond length = 0.776 Å
130 atoms, 168 bonds, 34 polyhedra; CPU time = 9 ms

130 atoms, 168 bonds, 34 polyhedra; CPU time = 9 ms

================================================================================
=
Title               Li4Ti2.5Ca2.5O12
```

```
Lattice type        F
Space group name    F d -3 m
Space group number  227
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 8.35700  8.35700  8.35700  90.0000  90.0000  90.0000

Unit-cell volume = 583.648349 Å^3

Structure parameters

                       x          y          z          Occ.     U    Site
Sym.
   1 Li  Li1         0.00000    0.00000    0.00000    1.000    0.000    8a      -
43m
   2 Ca  Ca2         0.62500    0.62500    0.62500    0.500    0.000   16d      .-
3m
   3 Ca  Ca1         0.62500    0.62500    0.62500    0.500    0.000   16d      .-
3m
   4 O   O1          0.38900    0.38900    0.38900    1.000    0.000   32e
.3m
================================================================================
=

Number of polygons and unique vertices on isosurface = 0 (0)
130 atoms, 168 bonds, 34 polyhedra; CPU time = 9 ms


POLYHEDRON:
   2     Ca2 Ca  0.12500  0.37500  0.87500  (-1, 1, 1)+ x+1/2, -y, -z+1/2
--------------------------------------------------------------------------------
   4      O1  O -0.11100  0.38900  0.88900  (-1, 0, 0)+ x+1/2, y, z+1/2
   4      O1  O  0.11100  0.38900  1.11100  ( 0, 0, 1)+ -x+1/2, y, -z+1/2
   4      O1  O  0.11100  0.61100  0.88900  ( 0, 1, 0)+ -y+1/2, -x, z+1/2
   4      O1  O  0.13900  0.13900  0.86100  (-1,-1, 1)+ y+3/4, x+3/4, -z+1/4
   4      O1  O  0.13900  0.36100  0.63900  (-1, 0, 0)+ x+3/4, -y+3/4, z+1/4
   4      O1  O  0.36100  0.36100  0.86100  ( 0, 0, 1)+ -y+3/4, -x+3/4, -z+1/4
--------------------------------------------------------------------------------

l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
----------------------------------------
Average bond length =  1.9792 Å
Polyhedral volume = 10.1251 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0139
Bond angle variance =  52.9620 deg.^2
Effective coordination number =  6.0000

Charge distribution
--------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
--------------------------------------------------------------------------------
                  x        y        z      delta_q    Q      q
   4      O1  O -0.11100  0.38900  0.88900    0.333 -1.250 -2.000
   4      O1  O  0.11100  0.38900  1.11100    0.333 -1.250 -2.000
   4      O1  O  0.11100  0.61100  0.88900    0.333 -1.250 -2.000
   4      O1  O  0.13900  0.13900  0.86100    0.333 -1.250 -2.000
   4      O1  O  0.13900  0.36100  0.63900    0.333 -1.250 -2.000
```

```
   4      O1  O  0.36100  0.36100  0.86100    0.333 -1.250 -2.000
-------------------------------------------------------------------------
   2     Ca2 Ca  0.12500  0.37500  0.87500           3.200  2.000

Input a bond valence parameter: 1.500000
Bond valence of O1: -0.273875
Bond valence of O1: -0.273875
Bond valence of O1: -0.273875
Bond valence of O1: -0.273875
Bond valence of O1: -0.273875
Bond valence of O1: -0.273875
Bond valence sum = 0.822
Oxidation state of the cation: +2
Expected bond length = 1.906 Å

POLYHEDRON:
   1     Li1 Li  0.50000  0.50000  1.00000  ( 0, 0, 1)+ -x+1/2, y+1/2, -z
-------------------------------------------------------------------------------
   4      O1  O  0.36100  0.36100  0.86100  ( 0, 0, 1)+ -y+3/4, -x+3/4, -z+1/4
   4      O1  O  0.36100  0.63900  1.13900  ( 0, 0, 0)+ -x+3/4, y+1/4, z+3/4
   4      O1  O  0.63900  0.36100  1.13900  ( 0, 0, 0)+ y+1/4, -x+3/4, z+3/4
   4      O1  O  0.63900  0.63900  0.86100  ( 0, 0, 1)+ x+1/4, y+1/4, -z+1/4
-------------------------------------------------------------------------------

l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
--------------------------------------
Average bond length =  2.0120 Å
Polyhedral volume =  4.1799 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0000
Bond angle variance =   0.0000 deg.^2
Effective coordination number =  4.0000

Charge distribution
-------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
-------------------------------------------------------------------------------
                   x        y        z      delta_q    Q      q
   4      O1  O  0.36100  0.36100  0.86100    0.250 -1.250 -2.000
   4      O1  O  0.36100  0.63900  1.13900    0.250 -1.250 -2.000
   4      O1  O  0.63900  0.36100  1.13900    0.250 -1.250 -2.000
   4      O1  O  0.63900  0.63900  0.86100    0.250 -1.250 -2.000
-------------------------------------------------------------------------------
   1     Li1 Li  0.50000  0.50000  1.00000           1.600  1.000

Input a bond valence parameter: 0.370000
Bond valence of O1: -0.0118218
Bond valence of O1: -0.0118218
Bond valence of O1: -0.0118218
Bond valence of O1: -0.0118218
Bond valence sum = 0.047
Oxidation state of the cation: +1
Expected bond length = 0.883 Å
OpenGL version: 4.6.14761 Compatibility Profile Context 21.30.44 30.0.13044.0
Video configuration: AMD Radeon(TM) Graphics
Maximum supported width and height of the viewport: 16384 x 16384
OpenGL depth buffer bit: 16
C:\Users\kiran kumar\Desktop\Li4Ti2.5Ca2.5O12.vesta
================================================================================
=
Title               Li4Ti2.5Ca2.5O12
Lattice type        F
Space group name    F d -3 m
```

```
Space group number  227
Setting number      1
Lattice parameters
   a        b        c       alpha    beta     gamma
 8.35700  8.35700  8.35700  90.0000  90.0000  90.0000

Unit-cell volume = 583.648349 Å^3
Structure parameters
                       x          y          z          Occ.     U    Site
Sym.
   1 Li  Li1          0.00000    0.00000    0.00000    1.000    0.000    8a      -
43m
   2 Ti  Ti2          0.62500    0.62500    0.62500    0.500    0.000   16d      .-
3m
   3 Ca  Ca1          0.62500    0.62500    0.62500    0.500    0.000   16d      .-
3m
   4 O   O1           0.38900    0.38900    0.38900    1.000    0.000   32e
.3m
================================================================================
=
Number of polygons and unique vertices on isosurface = 0 (0)
130 atoms, 168 bonds, 34 polyhedra; CPU time = 24 ms
POLYHEDRON:
   2     Ti2 Ti  0.62500  0.87500  0.87500  ( 1, 0, 0)+ -x+1/4, y+1/4, z+1/4
--------------------------------------------------------------------------------
   4      O1  O  0.38900  0.88900  0.88900  ( 0, 0, 0)+ x, y+1/2, z+1/2
   4      O1  O  0.63900  0.63900  0.86100  ( 0, 0, 1)+ x+1/4, y+1/4, -z+1/4
   4      O1  O  0.63900  0.86100  0.63900  ( 0, 1, 0)+ y+1/4, -x+1/4, z+1/4
   4      O1  O  0.61100  0.88900  1.11100  ( 1, 0, 1)+ -y, x+1/2, -z+1/2
   4      O1  O  0.61100  1.11100  0.88900  ( 1, 1, 0)+ -x, -y+1/2, z+1/2
   4      O1  O  0.86100  0.86100  0.86100  ( 1, 1, 1)+ -y+1/4, -x+1/4, -z+1/4
--------------------------------------------------------------------------------

l(Ti2-O1) =  1.97918(0) Å
l(Ti2-O1) =  1.97918(0) Å
l(Ti2-O1) =  1.97918(0) Å
l(Ti2-O1) =  1.97918(0) Å
l(Ti2-O1) =  1.97918(0) Å
l(Ti2-O1) =  1.97918(0) Å
---------------------------------------
Average bond length =  1.9792 Å
Polyhedral volume = 10.1251 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0139
Bond angle variance =  52.9620 deg.^2
Effective coordination number =  6.0000

Input a bond valence parameter: 0.370000
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence sum = 0.039
Oxidation state of the cation: +4
Expected bond length = 0.520 Å
106 atoms, 72 bonds, 18 polyhedra; CPU time = 6 ms

================================================================================
=
Title               Li4Ti2.5Ca2.5O12

Lattice type        F
Space group name    F d -3 m
Space group number  227
Setting number      1
```

```
Lattice parameters

   a        b        c       alpha    beta     gamma
 8.35700  8.35700  8.35700  90.0000  90.0000  90.0000

Unit-cell volume = 583.648349 Å^3

Structure parameters

                        x          y          z          Occ.     U    Site
Sym.
   1 Li  Li1          0.00000    0.00000    0.00000    1.000    0.000    8a      -
43m
   2 Ca  Ca2          0.62500    0.62500    0.62500    0.500    0.000   16d      .-
3m
   3 Ca  Ca1          0.62500    0.62500    0.62500    0.500    0.000   16d      .-
3m
   4 O   O1           0.38900    0.38900    0.38900    1.000    0.000   32e
.3m
================================================================================
=

Number of polygons and unique vertices on isosurface = 0 (0)
106 atoms, 72 bonds, 18 polyhedra; CPU time = 6 ms
106 atoms, 72 bonds, 18 polyhedra; CPU time = 6 ms
130 atoms, 168 bonds, 34 polyhedra; CPU time = 9 ms
130 atoms, 168 bonds, 34 polyhedra; CPU time = 9 ms
POLYHEDRON:
   2     Ca2 Ca  0.12500  0.37500  0.87500  (-1, 1, 1)+ x+1/2, -y, -z+1/2
--------------------------------------------------------------------------
   4      O1  O -0.11100  0.38900  0.88900  (-1, 0, 0)+ x+1/2, y, z+1/2
   4      O1  O  0.11100  0.38900  1.11100  ( 0, 0, 1)+ -x+1/2, y, -z+1/2
   4      O1  O  0.11100  0.61100  0.88900  ( 0, 1, 0)+ -y+1/2, -x, z+1/2
   4      O1  O  0.13900  0.13900  0.86100  (-1,-1, 1)+ y+3/4, x+3/4, -z+1/4
   4      O1  O  0.13900  0.36100  0.63900  (-1, 0, 0)+ x+3/4, -y+3/4, z+1/4
   4      O1  O  0.36100  0.36100  0.86100  ( 0, 0, 1)+ -y+3/4, -x+3/4, -z+1/4
--------------------------------------------------------------------------

l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
---------------------------------------
Average bond length =  1.9792 Å
Polyhedral volume = 10.1251 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0139
Bond angle variance =  52.9620 deg.^2
Effective coordination number =  6.0000
Input a bond valence parameter: 0.370000
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence sum = 0.039
Oxidation state of the cation: +2
Expected bond length = 0.776 Å

POLYHEDRON:
   2     Ca2 Ca  0.62500  0.87500  0.87500  ( 1, 0, 0)+ -x+1/4, y+1/4, z+1/4
--------------------------------------------------------------------------
   4      O1  O  0.38900  0.88900  0.88900  ( 0, 0, 0)+ x, y+1/2, z+1/2
   4      O1  O  0.63900  0.63900  0.86100  ( 0, 0, 1)+ x+1/4, y+1/4, -z+1/4
   4      O1  O  0.63900  0.86100  0.63900  ( 0, 1, 0)+ y+1/4, -x+1/4, z+1/4
```

```
   4      O1  O  0.61100  0.88900  1.11100  ( 1, 0, 1)+ -y, x+1/2, -z+1/2
   4      O1  O  0.61100  1.11100  0.88900  ( 1, 1, 0)+ -x, -y+1/2, z+1/2
   4      O1  O  0.86100  0.86100  0.86100  ( 1, 1, 1)+ -y+1/4, -x+1/4, -z+1/4
-------------------------------------------------------------------------------

l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
--------------------------------------
Average bond length =  1.9792 Å
Polyhedral volume = 10.1251 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0139
Bond angle variance =  52.9620 deg.^2
Effective coordination number =  6.0000

Input a bond valence parameter: 1.000000
Bond valence of O1: -0.0709036
Bond valence of O1: -0.0709036
Bond valence of O1: -0.0709036
Bond valence of O1: -0.0709036
Bond valence of O1: -0.0709036
Bond valence of O1: -0.0709036
Bond valence sum = 0.213
Oxidation state of the cation: +2
Expected bond length = 1.406 Å

POLYHEDRON:
   1     Li1 Li  0.50000  0.50000  1.00000  ( 0, 0, 1)+ -x+1/2, y+1/2, -z
-------------------------------------------------------------------------------
   4      O1  O  0.36100  0.36100  0.86100  ( 0, 0, 1)+ -y+3/4, -x+3/4, -z+1/4
   4      O1  O  0.36100  0.63900  1.13900  ( 0, 0, 0)+ -x+3/4, y+1/4, z+3/4
   4      O1  O  0.63900  0.36100  1.13900  ( 0, 0, 0)+ y+1/4, -x+3/4, z+3/4
   4      O1  O  0.63900  0.63900  0.86100  ( 0, 0, 1)+ x+1/4, y+1/4, -z+1/4
-------------------------------------------------------------------------------

l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
--------------------------------------
Average bond length =  2.0120 Å
Polyhedral volume =  4.1799 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0000
Bond angle variance =   0.0000 deg.^2
Effective coordination number =  4.0000


POLYHEDRON:
   1     Li1 Li  0.50000  0.50000  1.00000  ( 0, 0, 1)+ -x+1/2, y+1/2, -z
-------------------------------------------------------------------------------
   4      O1  O  0.36100  0.36100  0.86100  ( 0, 0, 1)+ -y+3/4, -x+3/4, -z+1/4
   4      O1  O  0.36100  0.63900  1.13900  ( 0, 0, 0)+ -x+3/4, y+1/4, z+3/4
   4      O1  O  0.63900  0.36100  1.13900  ( 0, 0, 0)+ y+1/4, -x+3/4, z+3/4
   4      O1  O  0.63900  0.63900  0.86100  ( 0, 0, 1)+ x+1/4, y+1/4, -z+1/4
-------------------------------------------------------------------------------
l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
--------------------------------------
Average bond length =  2.0120 Å
Polyhedral volume =  4.1799 Å^3
Distortion index (bond length) = 0.00000
```

```
Quadratic elongation =  1.0000
Bond angle variance =   0.0000 deg.^2
Effective coordination number =  4.0000

Input a bond valence parameter: 1.000000
Bond valence of O1: -0.064887
Bond valence of O1: -0.064887
Bond valence of O1: -0.064887
Bond valence of O1: -0.064887
Bond valence sum = 0.260
Oxidation state of the cation: +1
Expected bond length = 1.513 Å

POLYHEDRON:
   2     Ca2 Ca  0.12500  0.37500  0.87500  (-1, 1, 1)+ x+1/2, -y, -z+1/2
--------------------------------------------------------------------------
   4      O1  O -0.11100  0.38900  0.88900  (-1, 0, 0)+ x+1/2, y, z+1/2
   4      O1  O  0.11100  0.38900  1.11100  ( 0, 0, 1)+ -x+1/2, y, -z+1/2
   4      O1  O  0.11100  0.61100  0.88900  ( 0, 1, 0)+ -y+1/2, -x, z+1/2
   4      O1  O  0.13900  0.13900  0.86100  (-1,-1, 1)+ y+3/4, x+3/4, -z+1/4
   4      O1  O  0.13900  0.36100  0.63900  (-1, 0, 0)+ x+3/4, -y+3/4, z+1/4
   4      O1  O  0.36100  0.36100  0.86100  ( 0, 0, 1)+ -y+3/4, -x+3/4, -z+1/4
--------------------------------------------------------------------------
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
---------------------------------------
Average bond length = 1.9792 Å
Polyhedral volume = 10.1251 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation = 1.0139
Bond angle variance = 52.9620 deg.^2
Effective coordination number = 6.0000

POLYHEDRON:
   2     Ca2 Ca  0.62500  0.87500  0.87500  ( 1, 0, 0)+ -x+1/4, y+1/4, z+1/4
--------------------------------------------------------------------------
   4      O1  O  0.38900  0.88900  0.88900  ( 0, 0, 0)+ x, y+1/2, z+1/2
   4      O1  O  0.63900  0.63900  0.86100  ( 0, 0, 1)+ x+1/4, y+1/4, -z+1/4
   4      O1  O  0.63900  0.86100  0.63900  ( 0, 1, 0)+ y+1/4, -x+1/4, z+1/4
   4      O1  O  0.61100  0.88900  1.11100  ( 1, 0, 1)+ -y, x+1/2, -z+1/2
   4      O1  O  0.61100  1.11100  0.88900  ( 1, 1, 0)+ -x, -y+1/2, z+1/2
   4      O1  O  0.86100  0.86100  0.86100  ( 1, 1, 1)+ -y+1/4, -x+1/4, -z+1/4
--------------------------------------------------------------------------
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) = 1.97918(0) Å
---------------------------------------
Average bond length = 1.9792 Å
Polyhedral volume = 10.1251 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation = 1.0139
Bond angle variance = 52.9620 deg.^2
Effective coordination number = 6.0000

Input a bond valence parameter: 0.370000
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
Bond valence of O1: -0.012918
```

```
Bond valence sum = 0.039
Oxidation state of the cation: +2
Expected bond length = 0.776 Å
130 atoms, 168 bonds, 34 polyhedra; CPU time = 9 ms
130 atoms, 168 bonds, 34 polyhedra; CPU time = 9 ms
================================================================================
=
Title               Li4Ti2.5Ca2.5O12
Lattice type        F
Space group name    F d -3 m
Space group number  227
Setting number      1
Lattice parameters
 a        b        c       alpha    beta     gamma
 8.35700  8.35700  8.35700  90.0000  90.0000  90.0000
Unit-cell volume = 583.648349 Å^3
Structure parameters
                        x          y          z          Occ.     U    Site
Sym.
   1 Li  Li1          0.00000    0.00000    0.00000    1.000    0.000    8a      -
43m
   2 Ca  Ca2          0.62500    0.62500    0.62500    0.500    0.000   16d      .-
3m
   3 Ca  Ca1          0.62500    0.62500    0.62500    0.500    0.000   16d      .-
3m
   4 O   O1           0.38900    0.38900    0.38900    1.000    0.000   32e
.3m
================================================================================
=
Number of polygons and unique vertices on isosurface = 0 (0)
130 atoms, 168 bonds, 34 polyhedra; CPU time = 9 ms
POLYHEDRON:
   2     Ca2 Ca  0.12500  0.37500  0.87500  (-1, 1, 1)+ x+1/2, -y, -z+1/2
--------------------------------------------------------------------------------
   4      O1  O -0.11100  0.38900  0.88900  (-1, 0, 0)+ x+1/2, y, z+1/2
   4      O1  O  0.11100  0.38900  1.11100  ( 0, 0, 1)+ -x+1/2, y, -z+1/2
   4      O1  O  0.11100  0.61100  0.88900  ( 0, 1, 0)+ -y+1/2, -x, z+1/2
   4      O1  O  0.13900  0.13900  0.86100  (-1,-1, 1)+ y+3/4, x+3/4, -z+1/4
   4      O1  O  0.13900  0.36100  0.63900  (-1, 0, 0)+ x+3/4, -y+3/4, z+1/4
   4      O1  O  0.36100  0.36100  0.86100  ( 0, 0, 1)+ -y+3/4, -x+3/4, -z+1/4
--------------------------------------------------------------------------------

l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
l(Ca2-O1) =  1.97918(0) Å
----------------------------------------
Average bond length =  1.9792 Å
Polyhedral volume = 10.1251 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0139
Bond angle variance =  52.9620 deg.^2
Effective coordination number =  6.0000

Charge distribution
--------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
--------------------------------------------------------------------------------
                  x        y        z      delta_q    Q      q
   4      O1  O -0.11100  0.38900  0.88900    0.333 -1.250 -2.000
   4      O1  O  0.11100  0.38900  1.11100    0.333 -1.250 -2.000
   4      O1  O  0.11100  0.61100  0.88900    0.333 -1.250 -2.000
   4      O1  O  0.13900  0.13900  0.86100    0.333 -1.250 -2.000
   4      O1  O  0.13900  0.36100  0.63900    0.333 -1.250 -2.000
```

```
   4      O1  O  0.36100  0.36100  0.86100    0.333 -1.250 -2.000
-------------------------------------------------------------------------------
   2     Ca2 Ca  0.12500  0.37500  0.87500           3.200  2.000

Input a bond valence parameter: 1.500000
Bond valence of O1: -0.273875
Bond valence of O1: -0.273875
Bond valence of O1: -0.273875
Bond valence of O1: -0.273875
Bond valence of O1: -0.273875
Bond valence of O1: -0.273875
Bond valence sum = 0.822
Oxidation state of the cation: +2
Expected bond length = 1.906 Å

POLYHEDRON:
   1     Li1 Li  0.50000  0.50000  1.00000  ( 0, 0, 1)+ -x+1/2, y+1/2, -z
-------------------------------------------------------------------------------
   4      O1  O  0.36100  0.36100  0.86100  ( 0, 0, 1)+ -y+3/4, -x+3/4, -z+1/4
   4      O1  O  0.36100  0.63900  1.13900  ( 0, 0, 0)+ -x+3/4, y+1/4, z+3/4
   4      O1  O  0.63900  0.36100  1.13900  ( 0, 0, 0)+ y+1/4, -x+3/4, z+3/4
   4      O1  O  0.63900  0.63900  0.86100  ( 0, 0, 1)+ x+1/4, y+1/4, -z+1/4
-------------------------------------------------------------------------------

l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
---------------------------------------
Average bond length =  2.0120 Å
Polyhedral volume =  4.1799 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0000
Bond angle variance =   0.0000 deg.^2
Effective coordination number =  4.0000

Charge distribution
-------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
-------------------------------------------------------------------------------
                   x        y        z      delta_q    Q      q
   4      O1  O  0.36100  0.36100  0.86100    0.250 -1.250 -2.000
   4      O1  O  0.36100  0.63900  1.13900    0.250 -1.250 -2.000
   4      O1  O  0.63900  0.36100  1.13900    0.250 -1.250 -2.000
   4      O1  O  0.63900  0.63900  0.86100    0.250 -1.250 -2.000
-------------------------------------------------------------------------------
   1     Li1 Li  0.50000  0.50000  1.00000           1.600  1.000

Input a bond valence parameter: 0.370000
Bond valence of O1: -0.0118218
Bond valence of O1: -0.0118218
Bond valence of O1: -0.0118218
Bond valence of O1: -0.0118218
Bond valence sum = 0.047
Oxidation state of the cation: +1
Expected bond length = 0.883 Å
106 atoms, 72 bonds, 18 polyhedra; CPU time = 6 ms

106 atoms, 72 bonds, 18 polyhedra; CPU time = 6 ms

================================================================================
=
Title               Li4Ti2.5Cu2.5O12

Lattice type        F
Space group name    F d -3 m
```

```
Space group number  227
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 8.35700  8.35700  8.35700  90.0000  90.0000  90.0000

Unit-cell volume = 583.648349 Å^3

Structure parameters

                       x          y          z          Occ.     U    Site
Sym.
   1 Li  Li1         0.00000    0.00000    0.00000    1.000    0.000    8a      -
43m
   2 Cu  Cu2         0.62500    0.62500    0.62500    0.500    0.000   16d      .-
3m
   3 Cu  Cu1         0.62500    0.62500    0.62500    0.500    0.000   16d      .-
3m
   4 O   O1          0.38900    0.38900    0.38900    1.000    0.000   32e
.3m
================================================================================
=

Number of polygons and unique vertices on isosurface = 0 (0)
106 atoms, 72 bonds, 18 polyhedra; CPU time = 6 ms

130 atoms, 168 bonds, 34 polyhedra; CPU time = 9 ms

130 atoms, 168 bonds, 34 polyhedra; CPU time = 10 ms


POLYHEDRON:
   2     Cu2 Cu  0.12500  0.37500  0.87500  (-1, 1, 1)+ x+1/2, -y, -z+1/2
--------------------------------------------------------------------------------
   4      O1  O -0.11100  0.38900  0.88900  (-1, 0, 0)+ x+1/2, y, z+1/2
   4      O1  O  0.11100  0.38900  1.11100  ( 0, 0, 1)+ -x+1/2, y, -z+1/2
   4      O1  O  0.11100  0.61100  0.88900  ( 0, 1, 0)+ -y+1/2, -x, z+1/2
   4      O1  O  0.13900  0.13900  0.86100  (-1,-1, 1)+ y+3/4, x+3/4, -z+1/4
   4      O1  O  0.13900  0.36100  0.63900  (-1, 0, 0)+ x+3/4, -y+3/4, z+1/4
   4      O1  O  0.36100  0.36100  0.86100  ( 0, 0, 1)+ -y+3/4, -x+3/4, -z+1/4
--------------------------------------------------------------------------------

l(Cu2-O1) =  1.97918(0) Å
l(Cu2-O1) =  1.97918(0) Å
l(Cu2-O1) =  1.97918(0) Å
l(Cu2-O1) =  1.97918(0) Å
l(Cu2-O1) =  1.97918(0) Å
l(Cu2-O1) =  1.97918(0) Å
---------------------------------------
Average bond length =  1.992 Å
Polyhedral volume = 10.126 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.023
Bond angle variance =  52.9620 deg.^2
Effective coordination number =  6.0000

Charge distribution
--------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
--------------------------------------------------------------------------------
                  x        y        z      delta_q    Q      q
   4      O1  O -0.11100  0.38900  0.88900    0.333 -1.250 -2.000
   4      O1  O  0.11100  0.38900  1.11100    0.333 -1.250 -2.000
   4      O1  O  0.11100  0.61100  0.88900    0.333 -1.250 -2.000
```

```
   4      O1  O  0.13900  0.13900  0.86100    0.333 -1.250 -2.000
   4      O1  O  0.13900  0.36100  0.63900    0.333 -1.250 -2.000
   4      O1  O  0.36100  0.36100  0.86100    0.333 -1.250 -2.000
-------------------------------------------------------------------------------
   2     Cu2 Cu  0.12500  0.37500  0.87500           3.200  2.000

Input a bond valence parameter: 2.200000
Bond valence of O1: -1.81631
Bond valence of O1: -1.81631
Bond valence of O1: -1.81631
Bond valence of O1: -1.81631
Bond valence of O1: -1.81631
Bond valence of O1: -1.81631
Bond valence sum = 5.449
Oxidation state of the cation: +2
Expected bond length = 2.606 Å

POLYHEDRON:
   1     Li1 Li  0.50000  0.50000  1.00000  ( 0, 0, 1)+ -x+1/2, y+1/2, -z
-------------------------------------------------------------------------------
   4      O1  O  0.36100  0.36100  0.86100  ( 0, 0, 1)+ -y+3/4, -x+3/4, -z+1/4
   4      O1  O  0.36100  0.63900  1.13900  ( 0, 0, 0)+ -x+3/4, y+1/4, z+3/4
   4      O1  O  0.63900  0.36100  1.13900  ( 0, 0, 0)+ y+1/4, -x+3/4, z+3/4
   4      O1  O  0.63900  0.63900  0.86100  ( 0, 0, 1)+ x+1/4, y+1/4, -z+1/4
-------------------------------------------------------------------------------

l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
l(Li1-O1) =  2.01199(0) Å
---------------------------------------
Average bond length =  2.0130 Å
Polyhedral volume =  4.178 Å^3
Distortion index (bond length) = 0.00000
Quadratic elongation =  1.0000
Bond angle variance =   0.0000 deg.^2
Effective coordination number =  4.0000

Charge distribution
-------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
-------------------------------------------------------------------------------
                  x        y        z      delta_q    Q      q
   4      O1  O  0.36100  0.36100  0.86100    0.251 -1.250 -2.000
   4      O1  O  0.36100  0.63900  1.13900    0.251 -1.250 -2.000
   4      O1  O  0.63900  0.36100  1.13900    0.251 -1.250 -2.000
   4      O1  O  0.63900  0.63900  0.86100    0.251 -1.250 -2.000
-------------------------------------------------------------------------------
   1     Li1 Li  0.50000  0.50000  1.00000           1.600  1.000

Input a bond valence parameter: 0.370000
Bond valence of O1: -0.0118218
Bond valence of O1: -0.0118218
Bond valence of O1: -0.0118218
Bond valence of O1: -0.0118218
Bond valence sum = 0.047
Oxidation state of the cation: +1
Expected bond length = 0.883 Å
```

References

1. K.K. Surthi, K.K. Kar, Shape controlled and structurally stabilized Co-doped olivine lithium phosphate cathodes for high voltage conventional, thin and flexible Li-ion batteries, Chem. Eng. J. 399 (2020), 125858.

2. K.K. Surthi, A. Tyagi, K.K. Kar, First principle study on lithium-ion diffusion, electronic and electrochemical properties of cobalt doped lithium metal borates, J. Phys. Chem. Solid. 148 (2021), 109779.
3. K. K. Surthi, K. K. Kar, Spherical shaped $LiCo_{0.5}Mn_{0.5}PO_4$-carbon composite as high voltage cathode material for conventional and flexible Li-ion batteries, Carbon 193 (2022) 140-150
4. K.K. Surthi, K.K. Kar, Shape depended electrochemical properties of $LiNi_{0.5}Co_{0.5}PO_4$/C composites for high voltage secondary, flexible Li-ion batteries, Chem. Eng. J. 418 (2021), 129362.