# Supporting information for "Structural and thermodynamic properties of the $Li_6PS_5Cl$ solid electrolyte using first-principles calculations"

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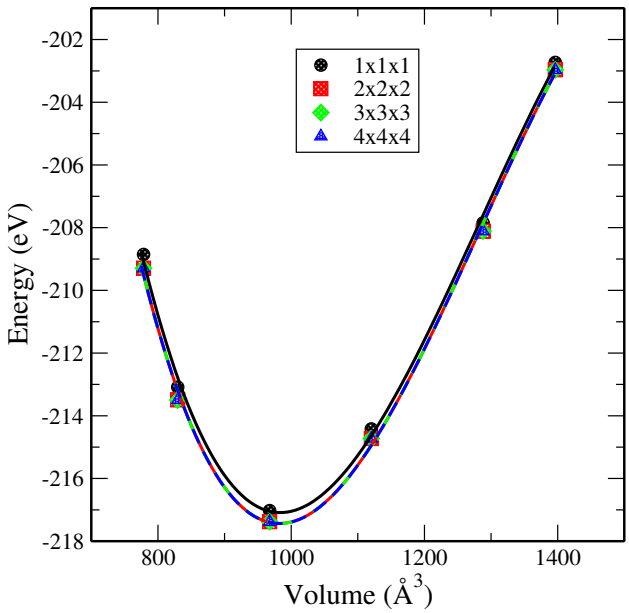


FIG. 1: Ground-state energy as a function of volume with different k-points grids, showing that the 1×1×1 grid, though not perfect for the total energy, gives correct equilibrium volume and bulk modulus.

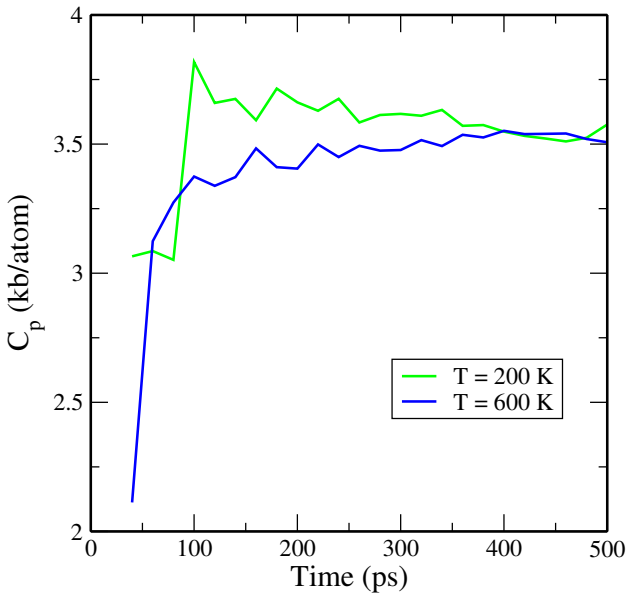


FIG. 2: Constant-pressure heat capacity $C_p = \left(\langle H^2\rangle_{t_{\rm sim}} - \langle H\rangle^2_{t_{\rm sim}}\right)/k_B T^2$ as a function of the total simulation time $t_{\rm sim}$. The equilibration period is kept fixed to 20 ps.

Here, we report the cif file of our best structure obtained at 0 K:

data_Li6PS5Cl

_symmetry_space_group_name_H-M 'P 1'

_cell_length_a 9.86406954

_cell_length_b 9.87240744

_cell_length_c 9.93943182

_cell_angle_alpha 90.00161132

_cell_angle_beta 90.15528498

_cell_angle_gamma 91.18990901

_symmetry_Int_Tables_number 1 _chemical_formula_structural Li6PS5Cl

_chemical_formula_sum 'Li24 P4 S20 Cl4'

_cell_volume 967.71059288

_cell_formula_units_Z 4

loop_

_symmetry_equiv_pos_site_id

_symmetry_equiv_pos_as_xyz

1 'x, y, z'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_symmetry_multiplicity

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

_atom_site_occupancy

Li Li0 1 0.97082601 0.82759174 0.15353743 1

Li Li1 1 0.06264261 0.88593683 0.80086287 1

Li Li2 1 0.02755084 0.19733758 0.22155313 1

Li Li3 1 0.33131115 0.19112378 0.48745550 1

Li Li4 1 0.82341978 0.51504197 0.70837821 1

Li Li5 1 0.46911868 0.68894462 0.86733139 1

Li Li6 1 0.45668585 0.96259279 0.70822551 1

Li Li7 1 0.96436680 0.26790402 0.59782647 1

Li Li8 1 0.19758249 0.53828079 0.70067028 1

Li Li9 1 0.71629085 0.51662740 0.21591435 1

Li Li10 1 0.66428743 0.80827283 0.49001516 1

Li Li11 1 0.94173384 0.69907764 0.41013500 1

Li Li12 1 0.18479862 0.45845674 0.35137748 1

Li Li13 1 0.71384027 0.70639875 0.01868709 1

Li Li14 1 0.68087924 0.98435941 0.29695005 1

Li Li15 1 0.21579178 0.17876007 0.01484801 1

Li Li16 1 0.65823707 0.17407130 0.54285645 1

Li Li17 1 0.30120289 0.47281188 0.08509362 1

Li Li18 1 0.33775043 0.02730790 0.28190497 1

Li Li19 1 0.31940788 0.82338635 0.50390804 1

Li Li20 1 0.51217238 0.70477090 0.20465834 1

Li Li21 1 0.82750831 0.17678527 0.95776320 1

Li Li22 1 0.53868573 0.35841642 0.85303306 1

Li Li23 1 0.49596511 0.31845854 0.19628440 1

P P24 1 0.00625979 -0.00942188 0.50278785 1

P P25 1 0.51427696 0.00843196 0.99473354 1

P P26 1 0.01418992 0.50613538 0.01917829 1

P P27 1 0.50388063 0.50107767 0.51900813 1

S S28 1 0.13081387 0.09537610 0.63264771 1

S S29 1 0.89313353 0.85322479 0.60980578 1

S S30 1 0.87997731 0.12653381 0.40670667 1

S S31 1 0.11887882 0.88953339 0.36113530 1

S S32 1 0.63678404 0.13020803 0.11388709 1

S S33 1 0.63274306 0.89343287 0.87090086 1

S S34 1 0.38146155 0.88474309 0.09553355 1

S S35 1 0.40799049 0.13672521 0.87116528 1

S S36 1 0.11671467 0.61629266 0.16476482 1

S S37 1 0.91891329 0.64594571 0.89902017 1

S S38 1 0.14691753 0.40035746 0.90130026 1

S S39 1 0.88344913 0.37088505 0.11046985 1

S S40 1 0.61410518 0.62669222 0.64535452 1

S S41 1 0.62866311 0.38261858 0.40534306 1

S S42 1 0.38393028 0.38055791 0.63970941 1

S S43 1 0.38095528 0.61291566 0.39542455 1

S S44 1 0.26296137 0.25642926 0.24702074 1

S S45 1 0.75380074 0.75565236 0.25914648 1

S S46 1 0.53259262 0.52199084 0.03688709 1

S S47 1 0.49719842 -0.00223135 0.47561085 1

Cl Cl48 1 0.76672849 0.27855181 0.74517104 1

Cl Cl49 1 0.27426550 0.76803378 0.73715831 1

Cl Cl50 1 0.01368816 0.02749686 0.00931053 1

Cl Cl51 1 0.01627135 0.49595769 0.53734121 1

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