Supplementary Information

Exploring ions migration in Li_2MnSiO_4 for Li-ion batteries through strain effect

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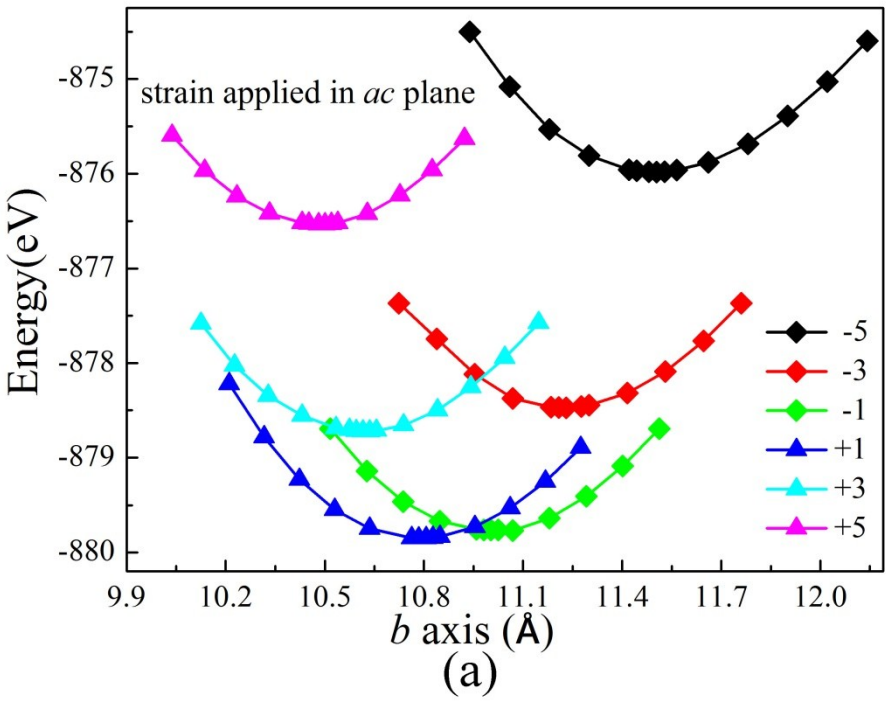
Table S1. Optimized lattice parameters for formula unit of Li_2MnSiO_4

Li_2MnSiO_4	a/ Å	b/ Å	c/ Å
Exp [1]	6.3109(9)	5.3800(9)	4.9662(8)
Thero[2]	6.468	5.429	5.039
Thero[3]	6.366	5.433	5.032
This work	6.3654	5.4247	5.0325



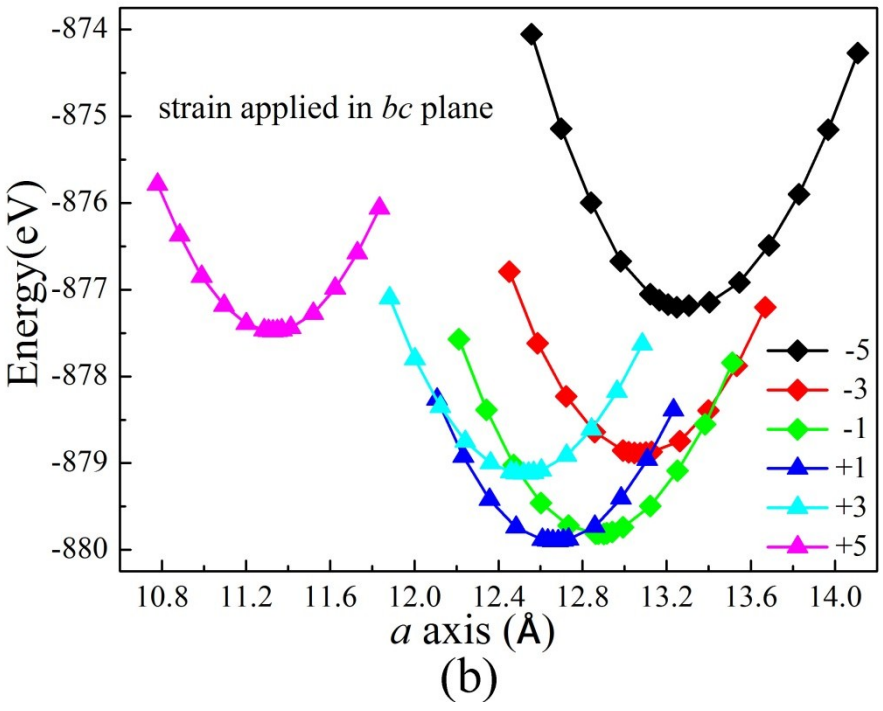
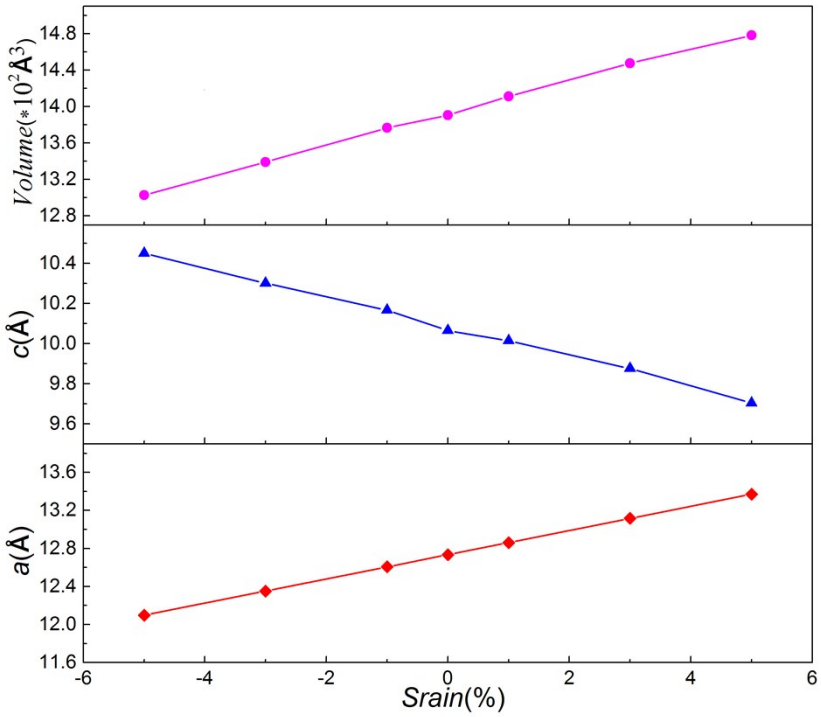
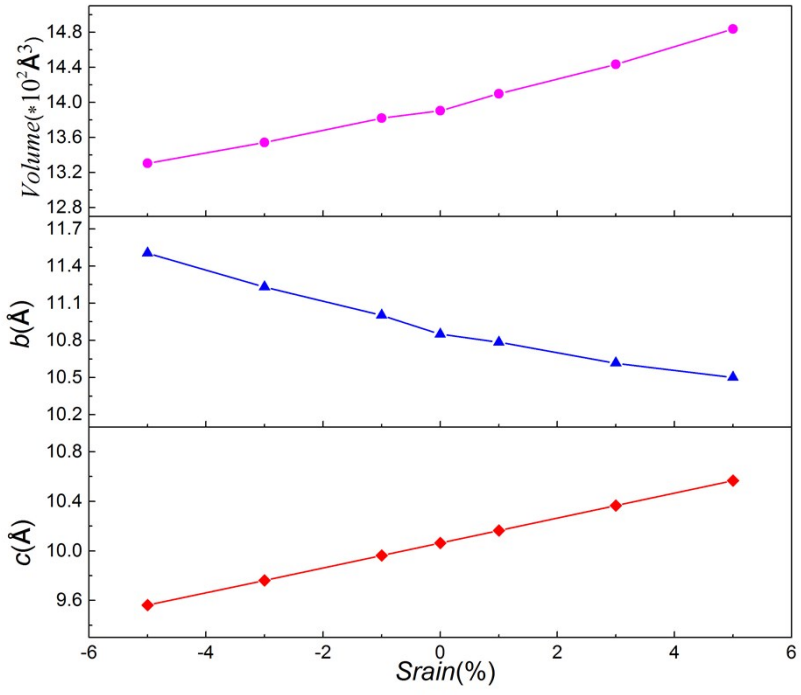


Figure S1 (a) Total energy for the suppercell (2×2×2) of Li_2MnSiO_4 as a function of the *b* axis lattice parameters for the different strain applied in the *ac* plane. (b) Total energy as a function of the *a* axis lattice parameters for the different strain applied in the *bc* plane. Here we also use two different accuracy values: 1% and 0.1%, so as to get the energy minimized structure. Comparing the energy for tensile and compressive strain, we can get the result that

the introduction of positive tensile strain is more favourable than compressive strain. The same conclusion as strain applied in *ab* plane.



(a)



(b)

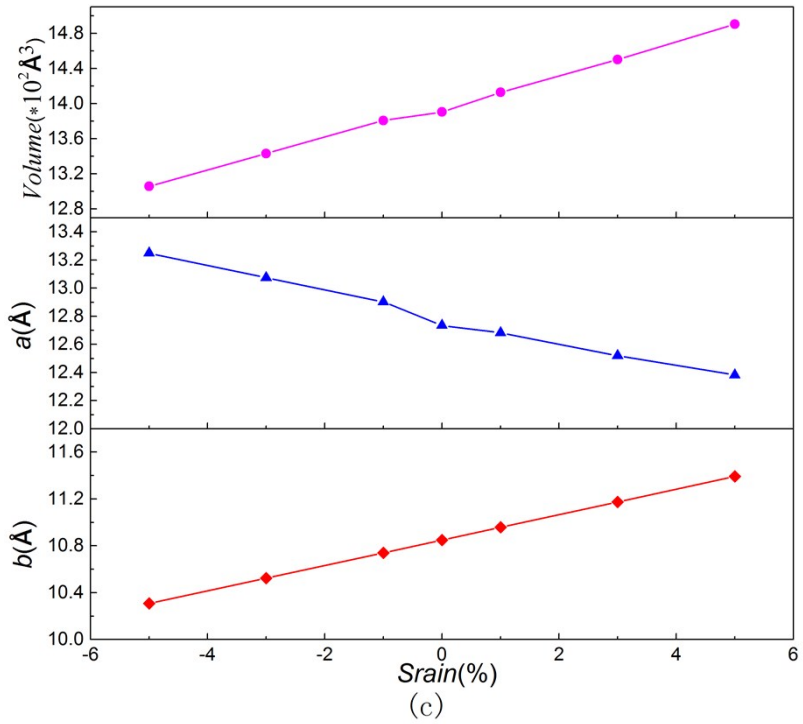


Figure S2. Calculate structure parameters and volume for Li_2MnSiO_4 structure under various applied biaxial strains in the (a) *ab* plane; (b) *ac* plane; (c) *bc* plane.

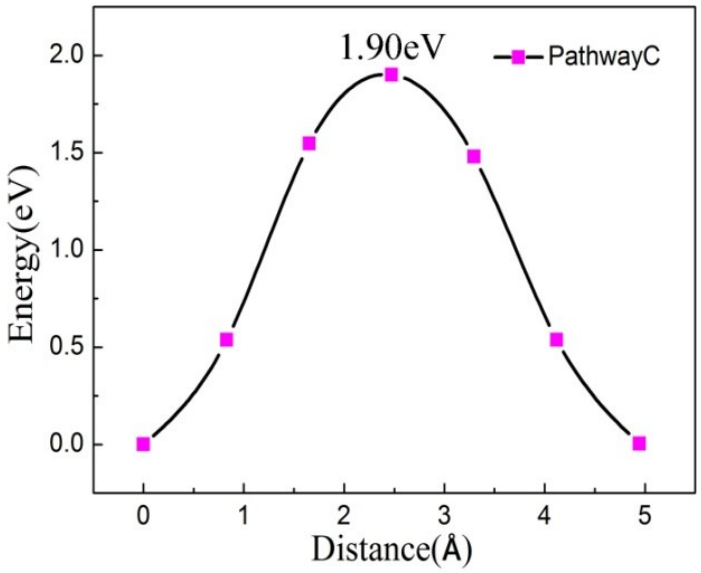


Figure S3. Calculate the activation barrier for pathway C. The migration is in the *bc* plane and across [MnSiO4] layer, when Li ion migration from pathway C the activation barrier is about

1.90 eV and jumping distance is 4.95 Å.

[1] Dominko R, Bele M, Gaberšček M, et al. Structure and electrochemical performance of Li 2 MnSiO 4 and Li 2 FeSiO 4 as potential Li-battery cathode materials[J]. Electrochemistry Communications, 2006, 8(2): 217-222.
[2] Lee H, Park S D, Moon J, et al. Origin of poor cyclability in Li2MnSiO4 from first-principles calculations: Layer exfoliation and unstable cycled structure[J]. Chemistry of Materials, 2014, 26(13): 3896-3899.
[3] Arroyo-deDompablo M E, Dominko R, Gallardo-Amores J M, et al. On the energetic stability and electrochemistry of Li2MnSiO4 polymorphs[J]. Chemistry of Materials, 2008, 20(17): 5574-5584.