Contribution ID: **264** Type: **Poster Presentation**

Ab initio studies on stabilities of products related to Li/S and Li/O batteries

Wednesday, 13 July 2011 17:00 (2 hours)

<p>Ab-intio Density Fuctional Theory has been employed to investigate the stabilities of Li< sub >2< /sub >O, Li< sub >2< /sub >S, Li< sub >2< /sub >O< sub >2< /sub > and Li< sub >2< /sub >S< sub >2< /sub > systems. Calculations were carried out utilizing Plane-wave Pseudopotential method within GGA-PBE using VASP CODE. We found good agreement between predicted data and experimental data of lattice parameters . The elastic constant for Li< sub >2< /sub >O, Li< sub >2< /sub >S accord well with experimental results and those of Li< sub >2< /sub >O< sub >2< /sub > and Li< sub >2< /sub >S< sub >2< /sub > are reasonably predicted, and satisfied stability conditions. Phonon dispersion of Li< sub >2< /sub >O and Li< sub >2< /sub >S compare well with those obtained from neutron scattering experiments. We predicted phonon dispersion of Li< sub >2< /sub >O< sub >2< /sub > suggest that the structure is stable, while those of Li< sub >2< /sub >S< sub >2< /sub >< sub >2< /sub > display soft modes along along Γ direction hence suggesting structural instabilities. Furthermore phonon density of states attribute the instability to the vibrations of the sulphur atoms in the ab plane.

Level (Hons, MSc,
   PhD, other)?

MSc

Consider for a student
   award (Yes / No)?

Yes

Would you like to <br> submit a short paper <br> for the Conference
 Proceedings (Yes / No)?

No

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