Supporting Information for "Enhanced Charge Transport in Amorphous Li_2O_2"

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Fig. S1 shows a histogram of the number of Li sites having coordination numbers ranging from 1 to 7. A significant fraction of Li sites are four- or five-fold coordinated.

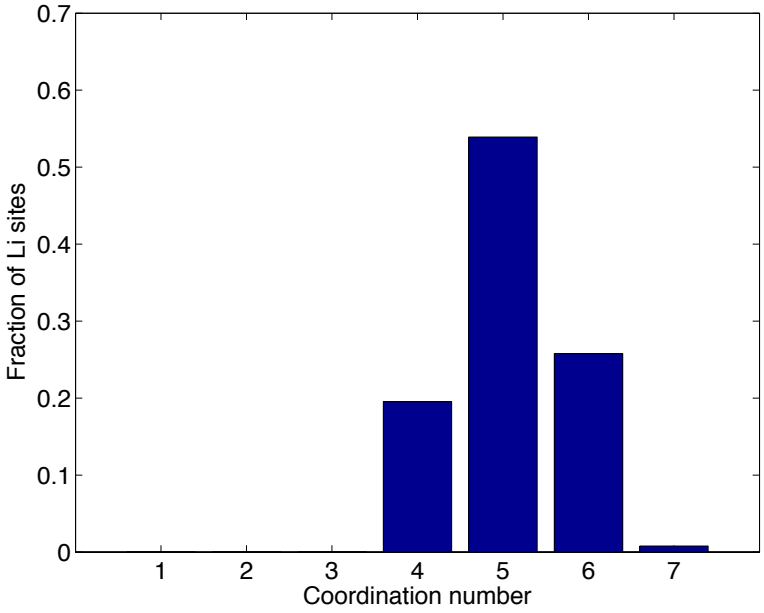

Figure S1. Li-O coordination number histogram for lithium sites in a-Li_2O_2 based on a 2.51 Å cutoff. In crystalline Li_2O_2, all Li sites have 6-fold coordination with oxygen.

Figs. S2, S3, S4, and S5 compare the defect formation and activation energies to various structural parameters measured in the PBE GGA defect-free amorphous cell. We did not find evidence for strong correlations between structural parameters and formation/activation energies. Note that both forwards and backwards barriers are included in Figs. S3, S4, and S5, so there are two points for every pathway.

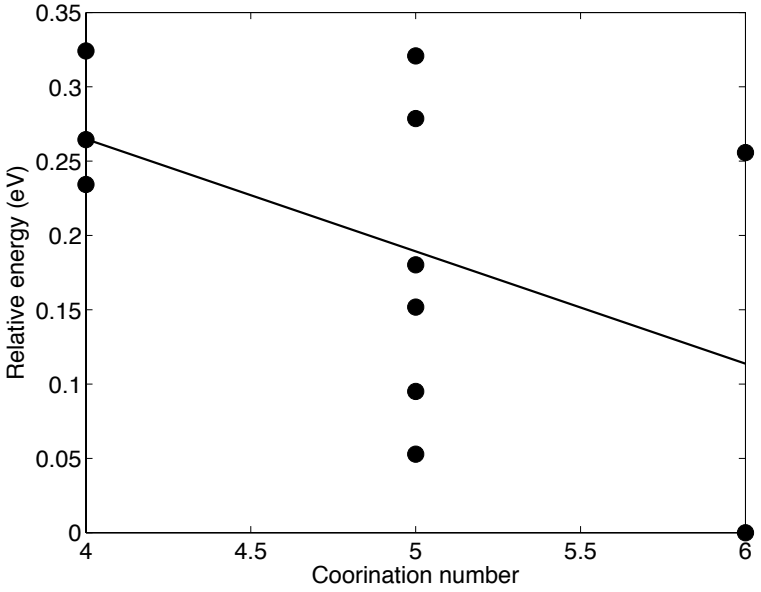

Figure S2. Relative HSE V_{Li}^{-} formation energies versus Li-O coordination number. The line shows a linear regression.

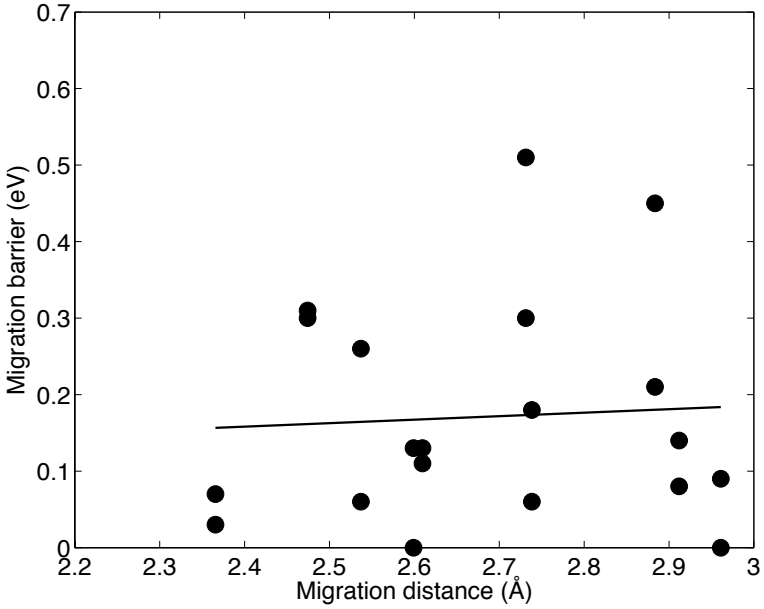

Figure S3. PBE GGA V_{Li}^{-} migration barriers versus migration distance. The line shows a linear regression.

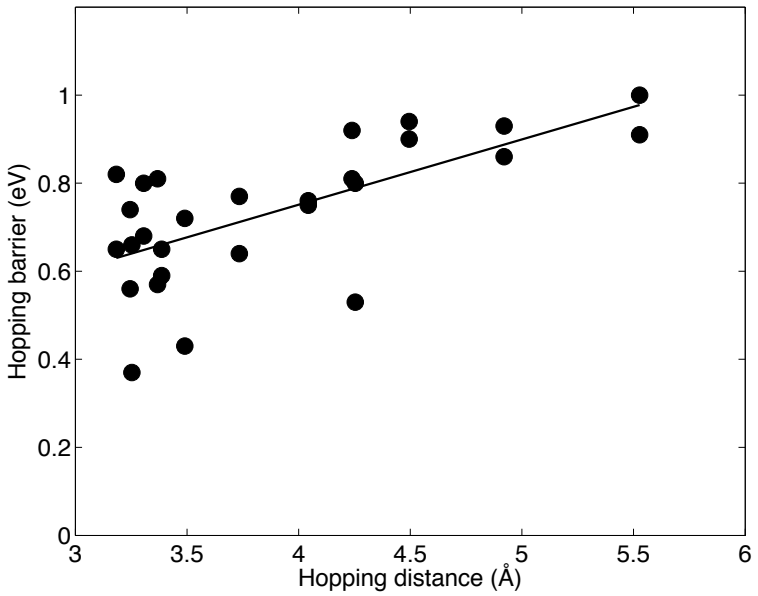

Figure S4. HSE hole polaron hopping barriers versus hopping distance, as measured between the centroids of the oxygen dimers. The line shows a linear regression.

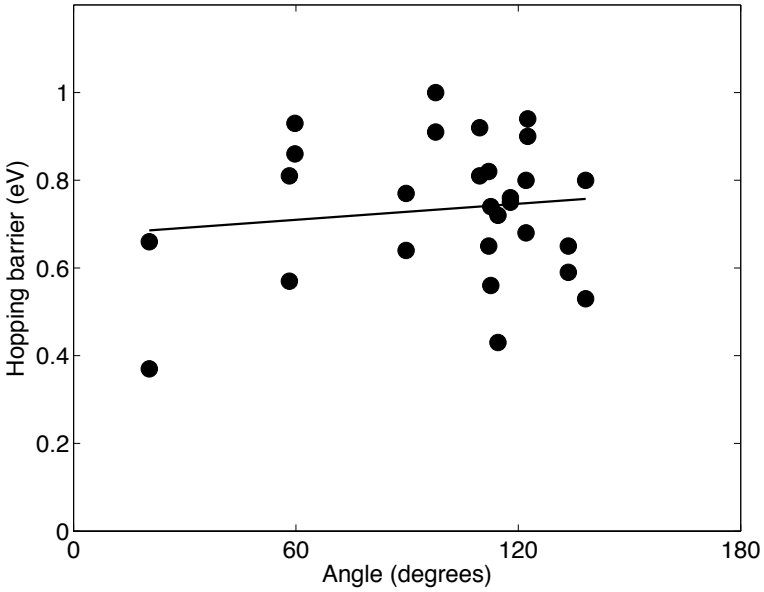

Figure S5. HSE hole polaron hopping barriers versus the angle between oxygen dimers. The line shows a linear regression.

Fig. S6 compares the HSE and PBE GGA formation energies of different Li sites relative to the most stable site. The fact that all of the points lie close to the line with slope one indicates that the two functionals agree well on the relative formation energies.

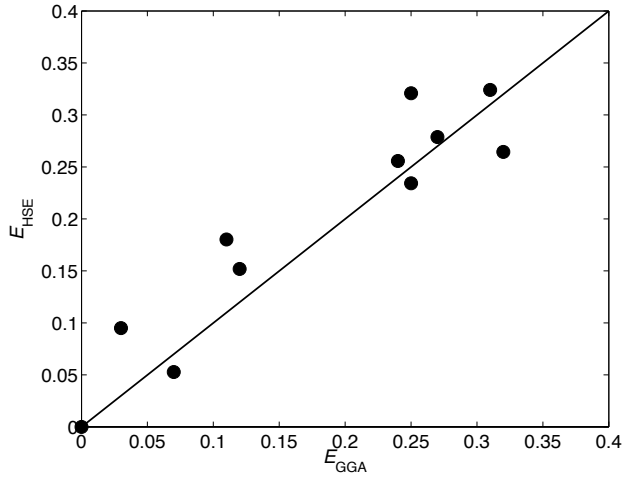

Figure S6. Comparison of the V_{Li}^{-} energies relative to the lowest energy site. The diagonal line has a slope of one.

Figs. S7 and S8 show histograms of the transition state energies $E_t = E_f + E_a$ for V_{Li}^- migration and p^+ hopping. The percolation thresholds, shown as vertical dashed lines, represent the 20th percentile of the transition state energies, calculated using linear interpolation.[1]

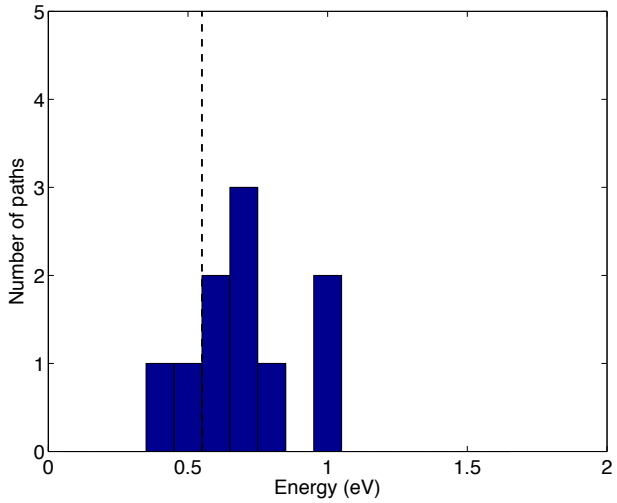

Figure S7. Histogram of transition state energies for V_{Li}^- migration. The vertical dashed line shows the calculated percolation energy.

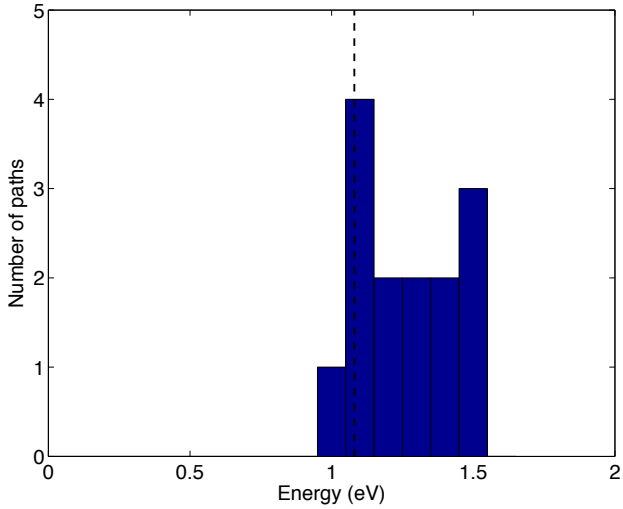

Figure S8. Histogram of transition state energies for p^+ hopping. The vertical dashed line shows the calculated percolation energy.

REFERENCES

(1) *Engineering statistics handbook*; NIST: Gaithersburg, MD, 2003.

The data below gives the atom positions (128 Li atoms, 128 O atoms, fractional coordinates) and unit cell geometry (in Angstroms) for amorphous Li_2O_2. The data is provided in VASP POSCAR format.

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   Li   O
   128   128
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