



Low Energy of Activation Lithium-Ion Conducting Channel

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Report Documentation Page

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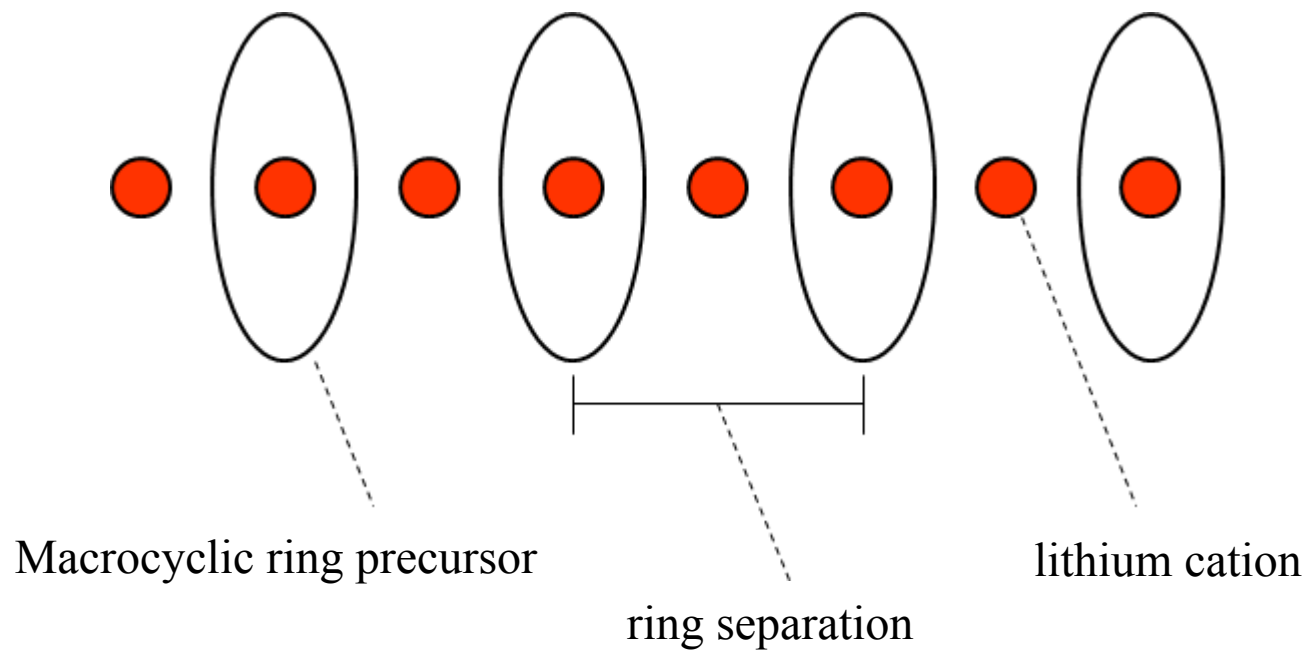
Outline



- **Lithium Ion Conducting Channel**
- **Negative Electrostatic Potential field**
 - Electron Delocalization
- **Low Energy of Activation**
 - Single Crystals
 - Thin Film
- **Conclusion**

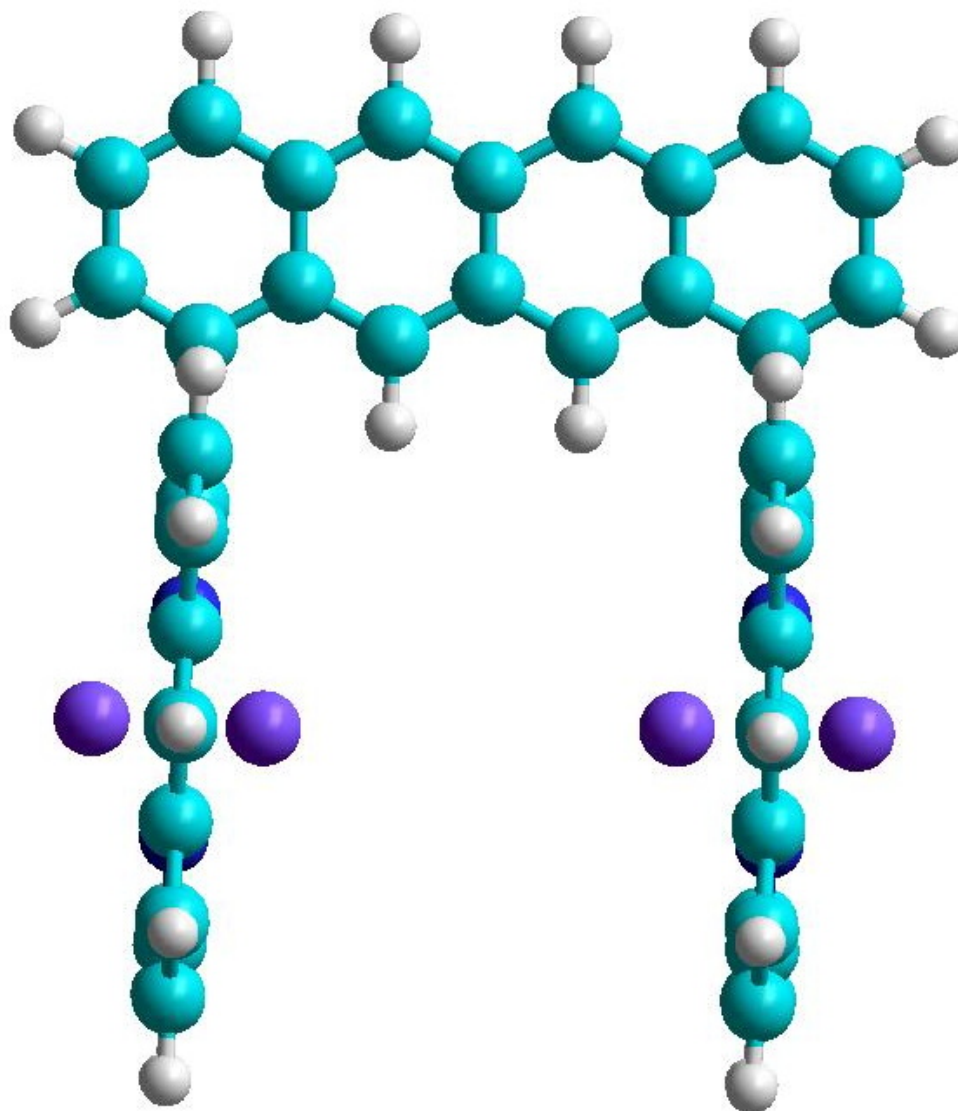


Conceptualized Lithium-Ion Conducting Channel



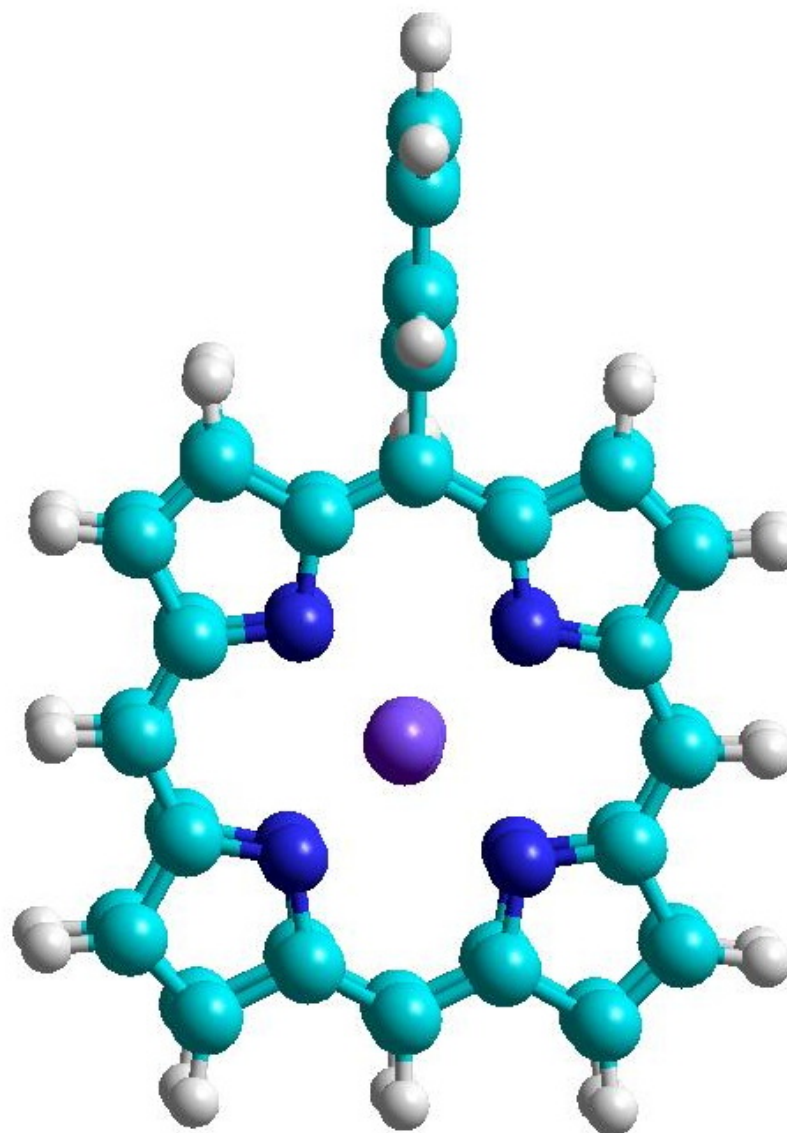


Channel Concept Based on Tetracene Bridging Unit with Dilithium Porphyrins Attached



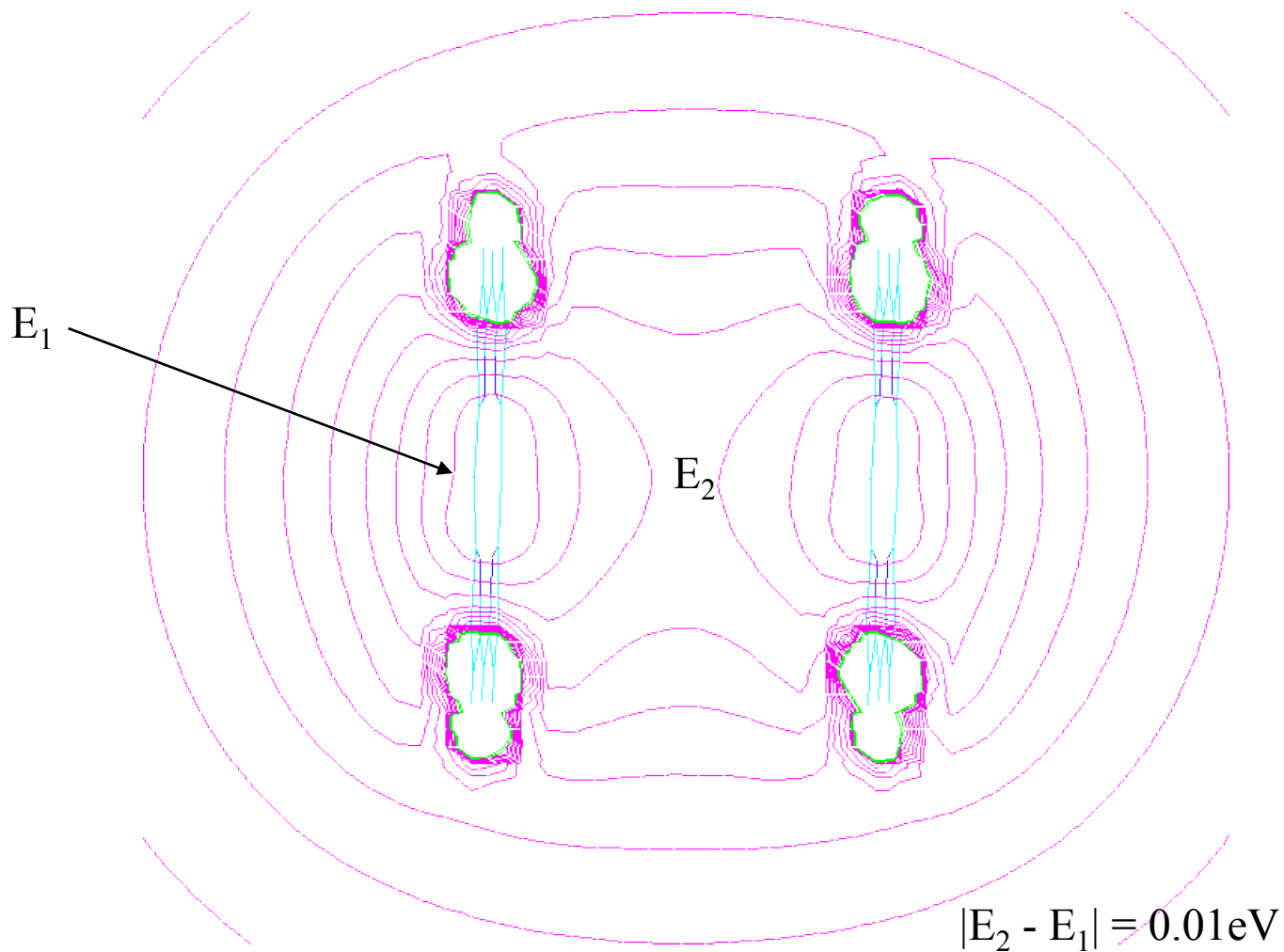


Channel Concept Based on Tetracene Bridging Unit with Dilithium Porphyrins Attached



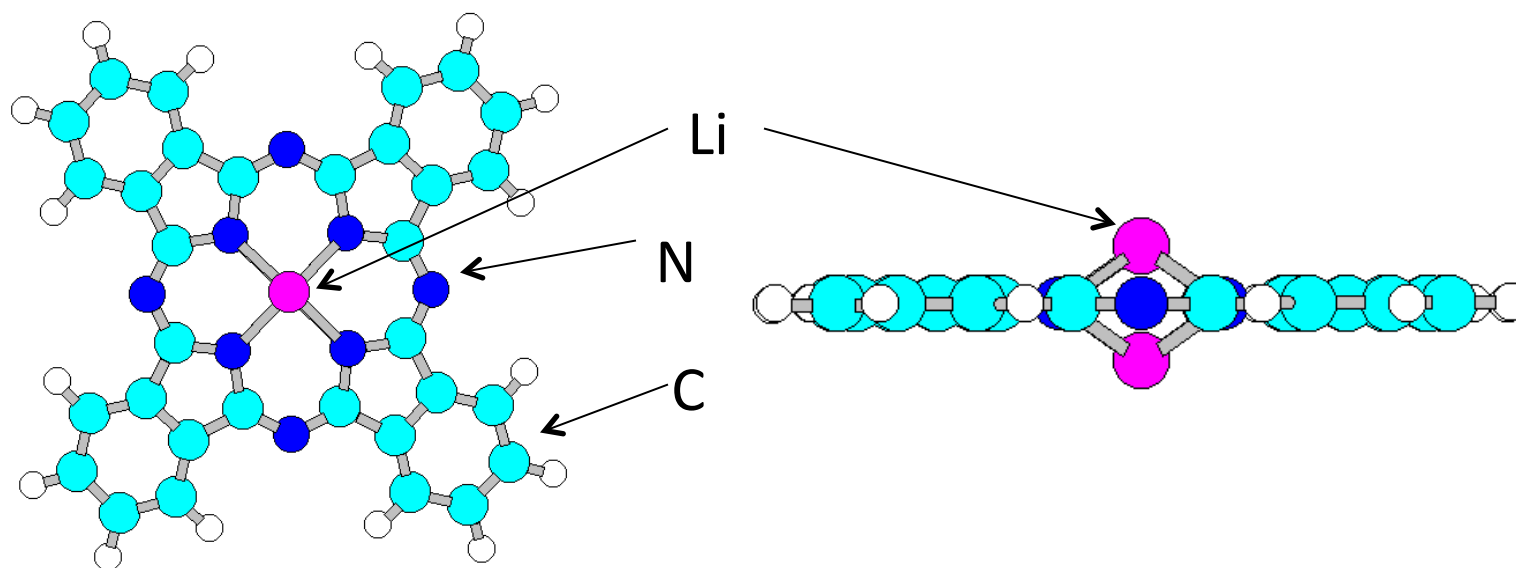


Negative Electrostatic Potential Contours for Two Porphyrin Dianions Separated by 7 Å. (E_2 , E_1 - Electrostatic Potential)



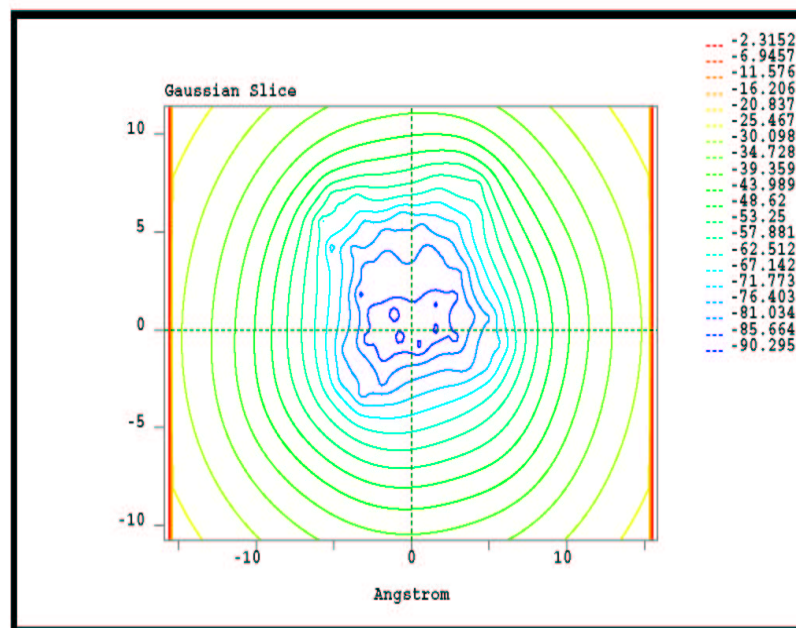
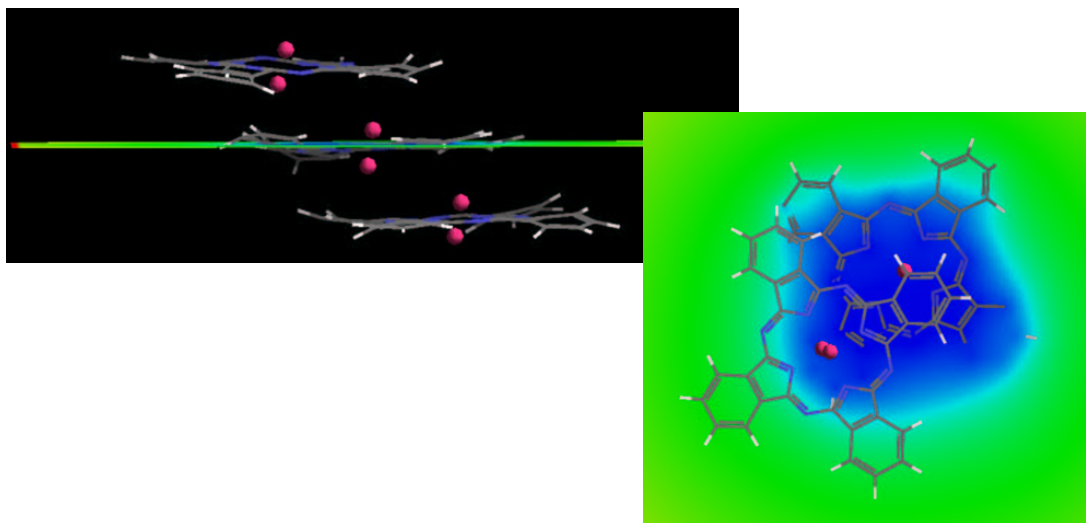


Dilithium Phthalocyanine (Li_2Pc)





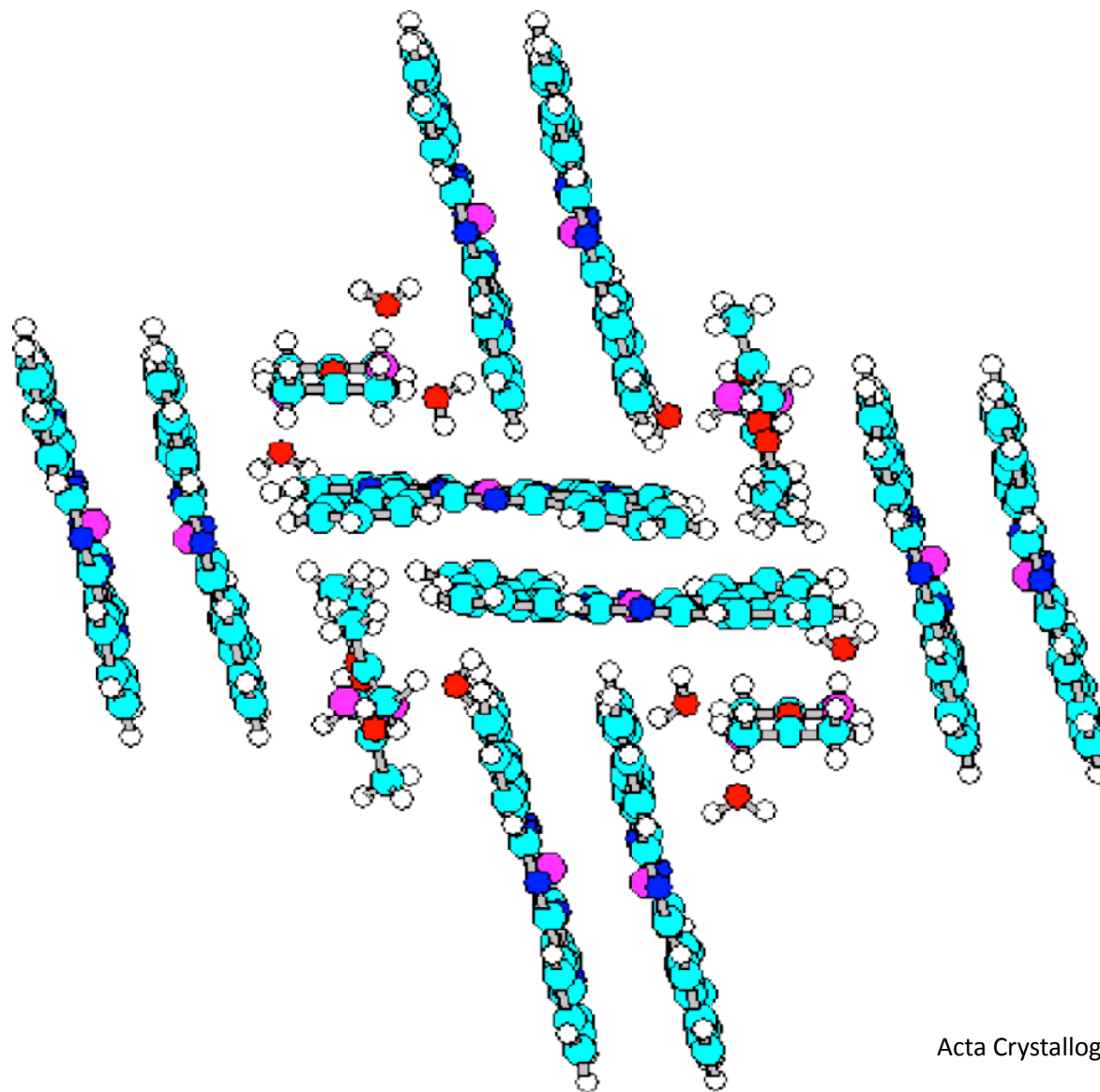
Calculated Electrostatic Potential Contours Obtained from Configurations Representative of Molecular Self-assembly of Li_2Pc Molecules; Side View (Above Left), Calculated Contours are for the Li_2Pc Molecule in the Middle; Profiles of Electrostatic Potential Contours as Viewed from the Top (Right and Below) of the Molecular System



J. Phys. Chem. B, 108, 4659 (2004)



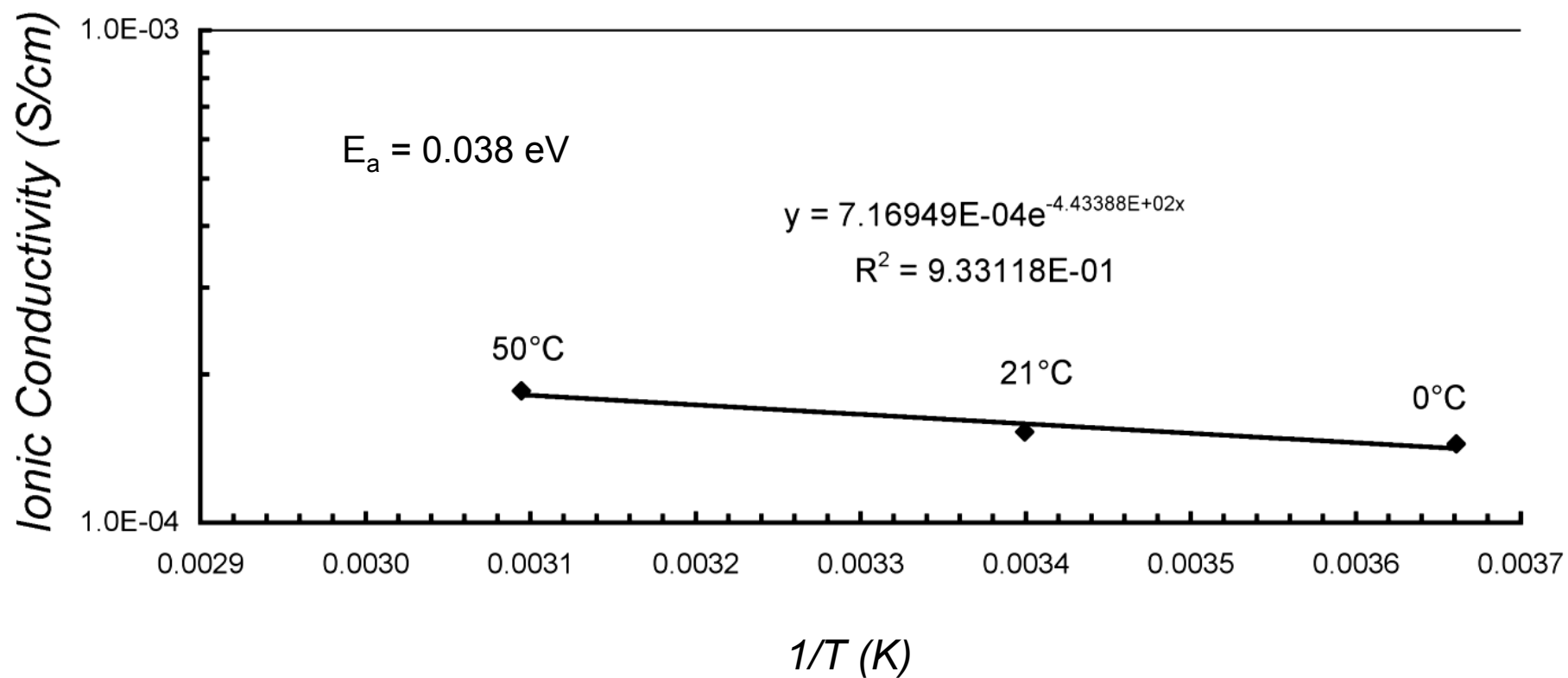
X-ray Crystal Structure of Li_2Pc



Acta Crystallogr. E62, m827-m829(2006)



Arrhenius Plot of Ionic Conductivity for a Pressed Pellet of Single Crystals of Li_2Pc Sandwiched Between Gold Electrodes ($710 \mu\text{m}$ Thick; 1.6 cm^2)

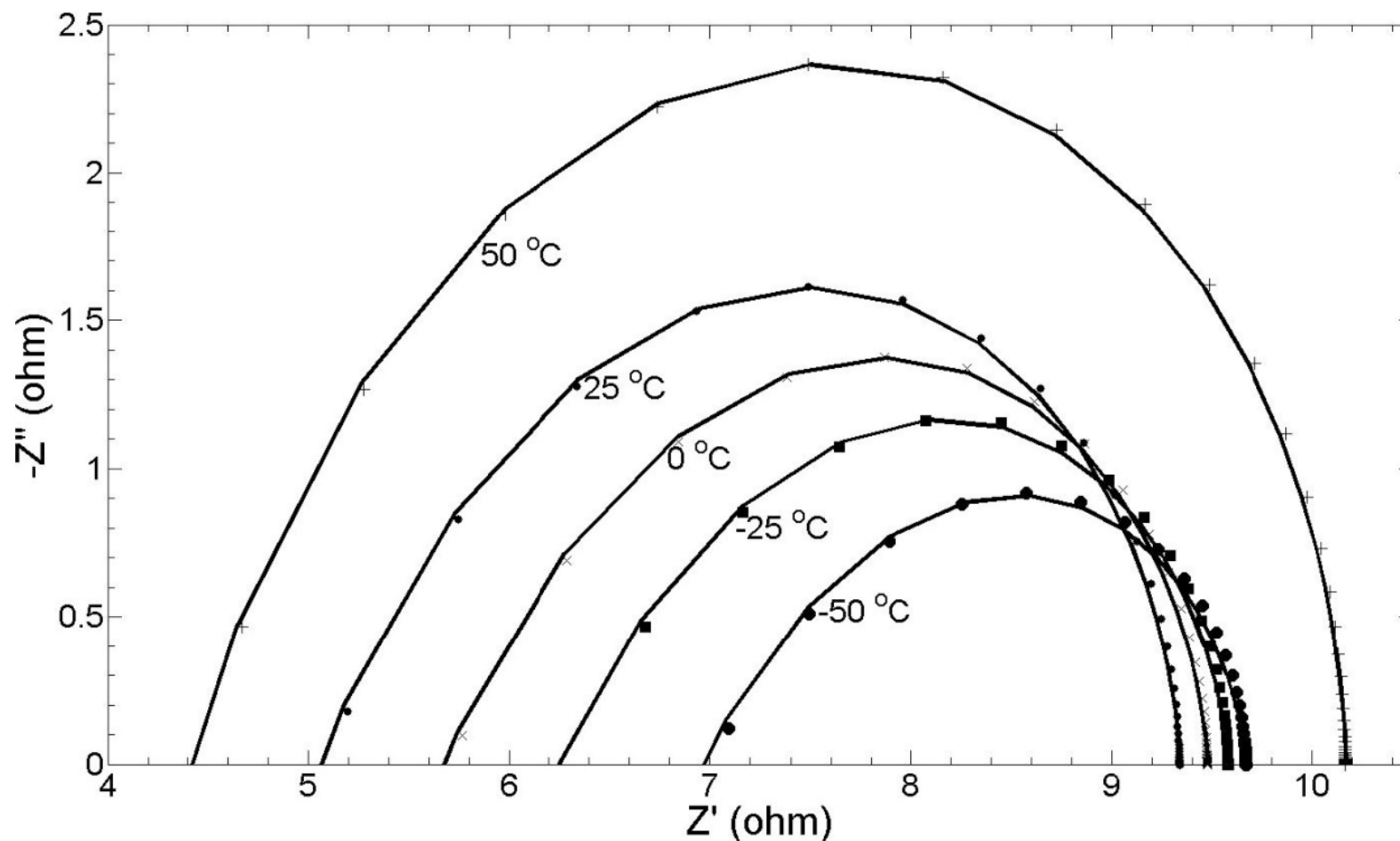


ECS Transactions, 25 (36) 163-167 (2010)

Electrochem. and Solid-State Letters, 8 (5), E45-E48 (2005)



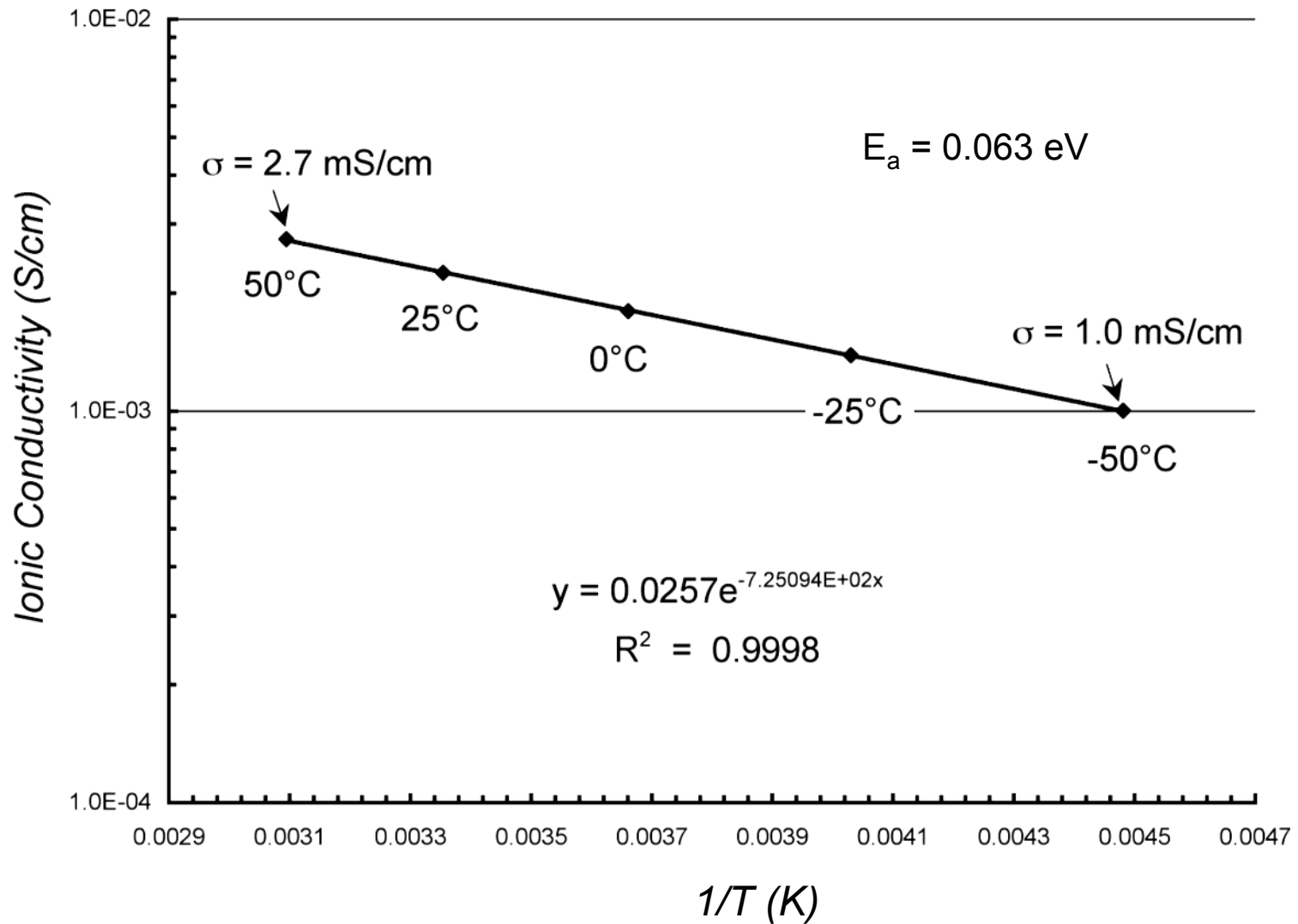
Nyquist Plots of SS/Thin Film Li_2Pc Cast Onto an MnO_2 Cathode/SS at $-50, -25, 0, +25,$ and 50°C



ECS Transactions, 25 (36) 163-167 (2010)



Arrhenius Plot of Ionic Conductivity for a Thin Film of Li_2Pc Cast Onto an MnO_2 Cathode at $-50, -25, 0, +25,$ and 50°C





Conclusions



The energies of activation for ionic conduction within the pressed pellet of single crystals (0.038 eV) and the thin film of Li_2Pc dried at 160°C (0.063 eV) would suggest a very similar conduction mechanism.

The lithium ion conduction pathway might be parallel to the a-axis between the phthalocyanine rings since there is a negative electrostatic potential field between the parallel phthalocyanine rings and in effect provides a constant sphere of solvation for the lithium ion throughout the crystal lattice.



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