

10<sup>TH</sup> ANNUAL  
CHEMISTRY & MASS SPECTROMETRY CONGRESS  
OCTOBER 18-19, 2017 OSAKA, JAPAN

**The effect of imidazole on the electrochemistry of zinc porphyrins: An electrochemical and computational study**

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In this study, the electrochemical behavior of zinc meso-substituted porphyrins in the presence of imidazole is examined by using both Cyclic Voltammetry (CV) and Density Functional Theory (DFT) methods. The results show that the first half-wave oxidation potentials ( $1^{\text{st}} E_{1/2}$ ) of zinc porphyrins complexed with imidazole all move to negative side while the second ones ( $2^{\text{nd}} E_{1/2}$ ) move positive side, resulting in larger half-wave oxidation potential splitting of the two oxidation states ( $\Delta E = \text{second } E_{1/2} - \text{first } E_{1/2}$ ) comparing with the zinc porphyrins. By employing DFT calculations, we have found that both sterically controlled inter  $\pi$ -conjugation between porphyrin rings and meso-substituted phenyl groups and deformation of porphyrin rings do play important roles in contributing to the half-wave oxidation potentials. Imidazole exhibits strong effects the deformation of porphyrin rings which determine the  $1^{\text{st}} E_{1/2}$  while inter  $\pi$ -conjugation between porphyrin rings and meso-substituted phenyl groups mainly contributes to the  $2^{\text{nd}} E_{1/2}$ . Without imidazole, inter  $\pi$ -conjugation between porphyrin rings and meso-substituted phenyl groups is the only important criterion which effects both  $1^{\text{st}} E_{1/2}$  and  $2^{\text{nd}} E_{1/2}$  of zinc porphyrins.

**Biography**

Yuhlong Oliver Su has completed his PhD at The Ohio State University and worked as Research Associate at Princeton University. He is currently the Professor of Chemistry and President of National Chi Nan University. He has published more than 82 papers in reputed journals.

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