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Computational and empiric considerations regarding electrocatalytic reduction of CO_2 by water soluble cobalt porphyrins

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The electrochemical reduction of CO_2 offers one of the possible solutions to current energy and sustainability issues since it can sequester carbon from the atmosphere and can be used to produce fuels and useful chemicals. In this respect, some metalloporphyrins have been reported to catalyze the electroreduction of CO_2. However, key issues still remain in regard to the elucidation of the effect of the porphyrin structure on the reaction mechanism and catalyst activity. An essential and necessary stage in the proposed mechanism for the catalytic reduction of CO_2 by the Co(II)/Co(I) porphyrin redox couple is the formation of an intermediate Co(II)porphyrin-CO_2- complex. In an attempt to examine the effect of positively and negatively charged porphyrin substituents on the catalytic activity, we report here on a combined DFT and empirical study regarding the electrochemical reduction of CO_2 in the presence of the Cobalt(II) 5,10,15,20-(tetra-N-methyl-4-pyridyl) porphyrin - Co(II) TMPyP and Cobalt(II) 5,10,15,20-(tetra-4-sulfonatophenyl) porphyrin – Co(II)TPPS complexes, with charges of +4 and -4, respectively. The lower catalytic activity of the CoTPPS complex as compared to that of CoTMPyP, both dissolved in aqueous alkaline solutions, as demonstrated by cyclic voltammetry experiments, are in agreement with the DFT study. Coulombic interactions seem to dictate the cobalt-carbon bond length and strength in the porphyrin-CO_2 intermediate, and consequently have an impact on its stability and on the overall catalytic activity towards CO_2 reduction.

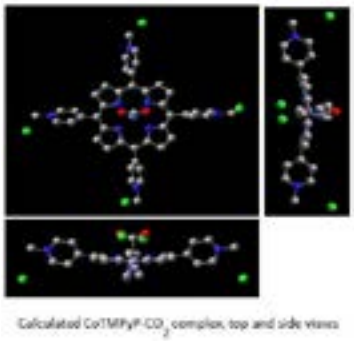

Figure 1: Calculated CoTMPyP-CO2 complex, top and side views.

Biography

Y Ben Eliyahu pursued all his degrees in Chemistry from the Hebrew University of Jerusalem, Jerusalem, Israel. His Msc and PhD theses were done under the supervision of the late Professor Yehuda Haas from the Physical Chemistry Department at the same university. He has been working in the Department of Chemistry Nuclear Research Center Negev (NRCN) since 1995; served as the Head of Department of Chemistry (2010-2013) at the same center. From 2013-2018 he became the Head of Nuclear Engineering Department of the Israel Atomic Energy Commission. Currently he is in sabbatical in the Department of Chemical Engineering at Ben Gurion University of the Negev (Israel).

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