



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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SHORT ABSTRACT

The prediction of efficiency is a challenging task. With the advent of computational modelling, reliable calculations can explain a quantitative aspect of the study. To acknowledge the efficiency of a catalyst, in the thesis, we formulated two models, viz. the efficiency conceptualization model (ECM) and the maximum kinetic efficiency (MaxKinEff) model for predicting the efficiencies of catalysts. The ECM is based upon the rate-determining step (RDS) of the reaction and considers its kinetic and thermodynamic aspects. On the other hand, MaxKinEff is a purely kinetic model that considers catalytic degradation in the catalytic cycle. With the obtained parameters, both models calculate the catalytic activity in terms of the turnover frequency (TOF). Further, we have deduced a formula for calculating the half-life of catalysts. Thus, using the value of TOF and half-life of catalysts, both models calculate the turnover number (TON) of catalysts under half-life conditions. The applicability of the two models has been tested with the twenty-six molecular water-oxidation catalysts (MWOCs) using the first, second, and third row transition metal catalysts. Both models conclude that the iridium-based MWOC shows a higher catalytic turnover number. The thesis finally provides a comparison of two established models.