Fen-Edebiyat Fakültesi
Kimya Bölümü
Faculty of Arts and Sciences
Department of Chemistry

Orta Doğu Teknik Üniversitesi
Middle East Technical University

Chemistry Department Seminar

Friday, 06.01.2023 at 15:40

Towards a Unified Computational Approach for Catalyst Identification and Discovery

Prof. Dr. Nihan Çelebi

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BS, Chemistry, Faculty of Science, Boğaziçi University
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PhD, Chemistry, Faculty of Science, Boğaziçi University, 2009
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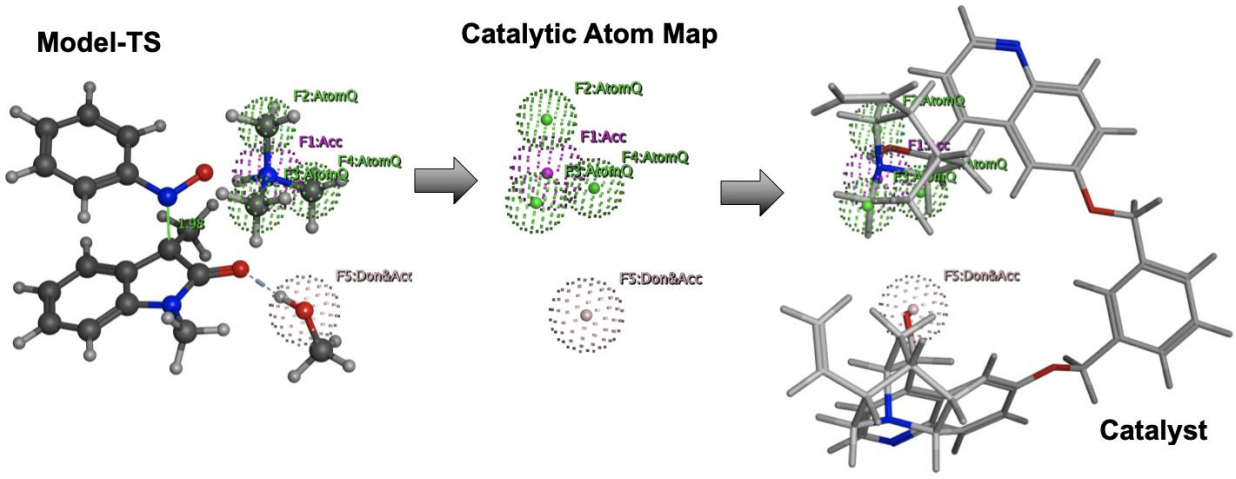
Abstract: Determination of efficient and selective catalytic structures still relies on an expensive and challenging method involving the synthesis of a large number of derivatives followed by experimental testing of their catalytic activities. A rational computational catalyst design approach could accelerate the discovery process. This lecture will describe how quantum mechanically optimized active site models are coupled with drug design tools to identify promiscuous enzyme activity for a chemical reaction not known in nature and to uncover new multifunctional catalysts that mimic the complex functional group assembly of enzyme active sites.



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