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

Orta Doğu Teknik Üniversitesi
Middle East Technical University

Chemistry Department Seminar

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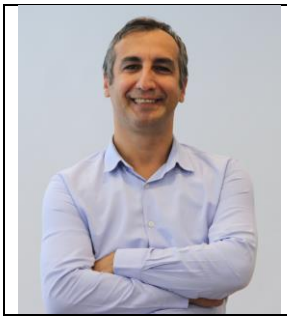
First Principle Calculations and Classical Molecular Dynamics Simulations on the Conducting Polymer-2D Material Nanocomposites

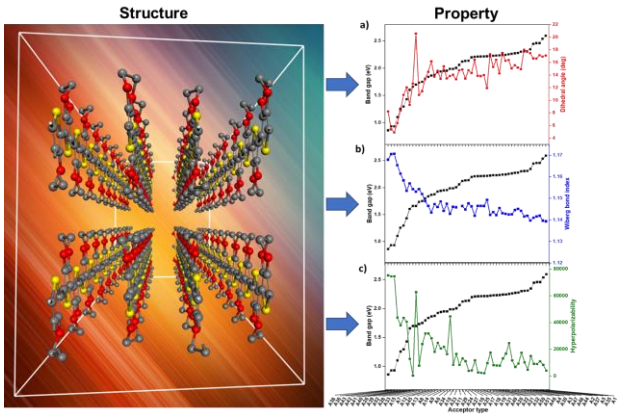


Asst. Prof. Erol Yıldırım

Chemistry Department, Faculty of Art and Sciences, METU

BS, Chemistry, Faculty of Science, İ.D. Bilkent University, 2003
MS, Chemistry, Institute of Sci. and Tech., İstanbul Teknik Üniversitesi, 2005
PhD, Chemistry, Institute of Sci. and Tech., İstanbul Teknik Üniversitesi, 2012
PostDoc, Aalto University, School of Chemical Technology, Finland, 2013-2015
PostDoc, North Carolina State Univ, Fiber and Polymer Science Program, USA 2015-2017
Research Scientist, Institute of High-Performance Computing, Singapore 2017-2019
Faculty, Chemistry Department, METU, 2019-Present

Abstract: Conducting polymer (CP)-2D material nanocomposites draw attention due to their enhanced physical, morphological and electrical properties which make them ideal candidates for organic electronics such as sensors, photovoltaic cells and energy storage materials. However, the origin of self-organization and self-alignment of CPs on the 2D surface is not known at molecular level that limit their electronic applications.



To understand the general rules for self-organization and self-alignment such as the presence of any directional preference of conducting polymers on the 2D materials such as graphene, graphene oxide and Mxene; first principle methods and molecular dynamics simulation studies were performed to determine general principles for the interaction of CPs including donor-acceptor conducting copolymers. To establish the principles of the self-organization on 2D materials, common CPs was selected from the experimental literature and structural optimizations were performed by using accurate first principle methods. The main parameters for the band gap engineering of donor and acceptor structures determined. We obtained wide range of differences for self-organization of different chains on the 2D surfaces. We showed that the origin of these structures is the ability of some CPs to position their electron rich aromatic centers with respect to the graphene carbons precisely. Due to this physical substrate effect, 2D materials can also improve the planarity and bond length alternation of CPs, which can lead to the optoelectronic performance improvement. These rules will help experimental researchers to tailor CP architecture which can result in the enhanced properties such as crystalline domains with high conductivity at the 2D-material interface.

Kimya Bölümü
Fen-Edebiyat Fakültesi
Orta Doğu Teknik Üniversitesi
06800 Ankara, Türkiye
kimya@metu.edu.tr

Department of Chemistry
Faculty of Arts and Sciences
Middle East Technical University
06800 Ankara, Turkey
kimya@metu.edu.tr