

## Asst. Prof. EROL YILDIRIM

### Personal Information

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### International Researcher IDs

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ScopusID: 16403972600

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### Education Information

Doctorate, Istanbul Technical University, Fen Bilimleri Enstitüsü, Chemistry, Turkey 2005 - 2012

Postgraduate, Istanbul Technical University, Fen Bilimleri Enstitüsü, Chemistry Program, Turkey 2004 - 2005

Undergraduate, Ihsan Dogramaci Bilkent University, Faculty Of Science, Chemistry, Turkey 1998 - 2003

### Foreign Languages

English, C2 Mastery

### Certificates, Courses and Trainings

Other, Reviewer Methods and Ethics Certificate, ACS Publications, 2018

### Dissertations

Doctorate, Molecular Dynamics Simulation Studies on the Physical Properties of Polyethylene-Organoclay Nanocomposite Materials, Istanbul Technical University, Fen Bilimleri Enstitüsü, Chemistry, 2012

Postgraduate, ACCURATE DETERMINATION OF THE POTENTIAL ENERGY SURFACES AND THE MOLECULAR PROPERTIES FOR  $MHe^+$  (M=Li, Na, K) COMPLEXES USING QUANTUM MECHANICAL TECHNIQUES, Istanbul Technical University, INSTITUTE OF SCIENCE AND TECHNOLOGY, 2005

### Research Areas

Chemistry

### Academic Titles / Tasks

Assistant Professor, Middle East Technical University, Faculty of Arts and Sciences, Department of Chemistry, 2019 - Continues

## Courses

Mathematics for Chemistry, Undergraduate, 2021 - 2022

Physical Chemistry II, Undergraduate, 2020 - 2021

General Chemistry, Undergraduate, 2020 - 2021

## Published journal articles indexed by SCI, SSCI, and AHCI

- I. **The impact of  $\pi$ -bridge moiety on the optoelectronic properties and photochemical stabilities of benzodithiophene-based conjugated polymers**  
DEMİR ARABACI E., Karakurt O., ÇIRPAN A., YILDIRIM E., ÖNAL A. M.  
Polymer, vol.313, 2024 (SCI-Expanded)
- II. **Design and performance of sulfur and selenium-substituted triarylboron D3-A TADF emitters for OLED applications**  
Karakurt O., Demirgezer E. F., DAŞTEMİR M., Cakmaktepe S. C., Miranda-Salinas H., Aksoy E., Danos A., Monkman A., YILDIRIM E., ÇIRPAN A.  
Organic Electronics, vol.134, 2024 (SCI-Expanded)
- III. **Design, Synthesis, and Theoretical Studies on the Benzoxadiazole and Thienopyrrole Containing Conjugated Random Copolymers for Organic Solar Cell Applications**  
Karakurt O., Oral P., Hacıoğlu S. O., Yılmaz E. A., Hacıfendioglu T., Bicer U. I., Ozcelik E., Ozsoy G. H., Yildirim E., Toppare L. K., et al.  
Macromolecular Rapid Communications, vol.45, no.19, 2024 (SCI-Expanded)
- IV. **Multiscale Modeling Approach to Understand Mechanism of Deposit Control by Sulfonate-Based Lubricant Detergents**  
Özdemir E., Kan E., Guo B., Pashkovski E., Agiral A., YILDIRIM E.  
ACS Omega, vol.9, no.37, pp.38753-38768, 2024 (SCI-Expanded)
- V. **Molecular Mechanism of Physical and Mechanical Improvement in Graphene/Graphene Oxide-Epoxy Composite Materials.**  
Budak D., Sarikurt S., Gur T., Ozkanakti H., Alagoz H., Eryol F., Yildirim E.  
Chemphyschem : a European journal of chemical physics and physical chemistry, 2024 (SCI-Expanded)
- VI. **Theoretical investigation on graphene induced self-alignment of donor-acceptor structures**  
Hacıfendioglu T., Aytemiz M. E., Korhan H., YILDIRIM E.  
Colloids and Surfaces A: Physicochemical and Engineering Aspects, vol.691, 2024 (SCI-Expanded)
- VII. **Influence of cationic dimeric and trimeric-type surfactants on the aggregation behavior of water-soluble phthalocyanine: A combined experimental and computational study**  
El-Khouly M. E., El-Said W. A., Yildirim E., El-Shafei A.  
Journal of Molecular Liquids, vol.400, 2024 (SCI-Expanded)
- VIII. **How do we get across? Impact of bridging aromatic units on the optical, electronic, and photovoltaic properties of donor-acceptor polymers**  
Dikbiyik D. E., Karakurt O., Cevher D., Ozsoy G. H., Yildirim E., Cirpan A.  
Polymer, vol.294, 2024 (SCI-Expanded)
- IX. **Two-Dimensional TiS<sub>2</sub> Nanosheet- and Conjugated Polymer Nanoparticle-Based Composites for Sensing Applications**  
Yeniterzi D., Cevher S., Kandur Baglicakoglu S., Ucar A., DURUKAN M. B., Hacıfendioglu T., YILDIRIM E., ÇIRPAN A., ÜNALAN H. E., Soylemez S.  
Langmuir, 2024 (SCI-Expanded)

- X. **Theoretical and experimental investigation of bridging atom effect on the fluorene and silafluorene based trimeric monomers and their corresponding polymers**  
DEMİR ARABACI E., YILDIRIM E., ÖNAL A. M.  
Dyes and Pigments, vol.216, 2023 (SCI-Expanded)
- XI. **Effect of phthalimide and thieno[3,4-c]pyrrole-4,6,dione acceptors on  $\pi$ -conjugated donor-acceptor-donor monomers: Experimental and theoretical investigations of photophysical and electrochemical properties**  
ÇAKAL D., DEMİR ARABACI E., YILDIRIM E., Cihaner A., ÖNAL A. M.  
Tetrahedron, vol.140, 2023 (SCI-Expanded)
- XII. **Low-cost novel X-shaped hole transport materials for efficient perovskite solar cells: Molecular modelling of the core and schiff base effects on photovoltaic and photophysical properties**  
Abdellah I. M., YILDIRIM E., El-Shafei A.  
Materials Chemistry and Physics, vol.296, 2023 (SCI-Expanded)
- XIII. **Side chain effect on the electrochemical and optical properties of thieno[3,4-c]pyrrole-4,6-dione based donor-acceptor donor type monomers and polymers**  
ÇAKAL D., DEMİR ARABACI E., YILDIRIM E., CİHANER A., ÖNAL A. M.  
MOLECULAR SYSTEMS DESIGN & ENGINEERING, vol.8, no.1, pp.65-78, 2023 (SCI-Expanded)
- XIV. **Roadmap to Design Mechanically Robust Copolymer Hydrogels Naturally Cross-Linked by Hydrogen Bonds**  
Erkoc C., YILDIRIM E., Yurtsever M., Okay O.  
Macromolecules, vol.55, no.23, pp.10576-10589, 2022 (SCI-Expanded)
- XV. **Organic Charge Transfer Cocrystals as Additives for Dissipation of Contact Charges on Polymers**  
Ekim S. D., Kaya G. E., DAŞTEMİR M., YILDIRIM E., BAYTEKİN H. T., BAYTEKİN B.  
ACS APPLIED MATERIALS & INTERFACES, vol.14, no.50, pp.56018-56026, 2022 (SCI-Expanded)
- XVI. **Rational Molecular Design Enables Efficient Blue TADF–OLEDs with Flexible Graphene Substrate**  
Sharif P., Alemdar E., Ozturk S., Caylan O., Hacıfendioglu T., Buke G., Aydemir M., Danos A., Monkman A. P., Yildirim E., et al.  
Advanced Functional Materials, vol.32, no.47, 2022 (SCI-Expanded)
- XVII. **Organocatalytic enantioselective synthesis of dihydronaphthofurans and dihydrobenzofurans: reaction development and insights into stereoselectivity**  
SUSAM Z. D., Ozcan B. D., Kurtkaya E., YILDIRIM E., TANYELİ C.  
ORGANIC & BIOMOLECULAR CHEMISTRY, vol.20, no.44, pp.8725-8740, 2022 (SCI-Expanded)
- XVIII. **Design Principles for the Acceptor Units in Donor-Acceptor Conjugated Polymers**  
Hacıfendioglu T., YILDIRIM E.  
ACS OMEGA, vol.7, no.43, pp.38969-38978, 2022 (SCI-Expanded)
- XIX. **Investigation the effect of  $\pi$  bridge and side chain on photovoltaic properties of benzodithiophene and quinoxaline based conjugated polymers**  
TAŞKAYA ASLAN S., Alemdar Yılmaz E., Hacıfendioglu T., UDUM Y., TOPPARE L. K., YILDIRIM E., ÇIRPAN A.  
European Polymer Journal, vol.169, 2022 (SCI-Expanded)
- XX. **Synthesis of a Novel and More Sustainable Cationic Bleach Activator, N-[4-(N, N, N)-Triethylammoniumchloride-butanoyl] Butyrolactam, for Cotton: Optimization and Theoretical Limitations**  
Altay P., Yildirim E., Gürsoy N. Ç., Hauser P. J., El-Shafei A.  
ACS Sustainable Chemistry and Engineering, vol.10, no.14, pp.4415-4424, 2022 (SCI-Expanded)
- XXI. **A Dual-Surface Mechanism of Oxidant-Free Pyrrole Polymerization in the Two-Dimensional Titanium Carbide (MXene) Interlayer Nanospace**  
YILDIRIM E., Goh S. S., Luo H., Jin H., Wu G., Tan T. L., Wong Z. M., Xu J., Yang S.  
JOURNAL OF PHYSICAL CHEMISTRY C, vol.126, no.3, pp.1316-1325, 2022 (SCI-Expanded)
- XXII. **Boron Cage Triggered Micellization of a Neutral-Cationic Block Copolymer and Preparation of Boron-Containing Layer-by-Layer Microparticles**  
Aydemir U., Ugur E., Ermis C., Aydemir F. N., Ozdemir E., Banerjee S., Yildirim E., Akdağ A., Erel Göktepe I.

- ACS Applied Polymer Materials, vol.4, no.5, pp.3448-3461, 2022 (SCI-Expanded)
- XXIII. **Hydrolytic Degradation of Polylactic Acid Fibers as a Function of pH and Exposure Time**  
Vaid R., Yildirim E., Pasquinelli M. A., King M. W.  
MOLECULES, vol.26, no.24, 2021 (SCI-Expanded)
- XXIV. **Mechanically robust hybrid hydrogels of photo-crosslinkable gelatin and laminin-mimetic peptide amphiphiles for neural induction**  
Isik M., Eylem C. C., Hacıfendioglu T., YILDIRIM E., Sari B., NEMUTLU E., EMREGÜL E., Okesola B. O., DERKUŞ B.  
BIOMATERIALS SCIENCE, vol.9, no.24, pp.8270-8284, 2021 (SCI-Expanded)
- XXV. **Synthesis of selenophene substituted benzodithiophene and fluorinated benzothiadiazole based conjugated polymers for organic solar cell applications**  
TAŞKAYA ASLAN S., Cevher D., Bolayır E., Hizalan Ozsoy G., UDUM Y., YILDIRIM E., TOPPARE L. K., ÇIRPAN A.  
Electrochimica Acta, vol.398, 2021 (SCI-Expanded)
- XXVI. **Effect of thiophene, 3-hexylthiophene, selenophene, and Thieno[3,2-b] thiophene spacers on OPV device performance of novel 2,1,3-benzothiadiazole based alternating copolymers**  
Karaman C. Z., Goker S., Sahin U. S., Hacıoglu Ş., Aslan S. T., Hacıfendioglu T., Hizalan G., YILDIRIM E., ÇIRPAN A., TOPPARE L. K.  
JOURNAL OF ELECTROANALYTICAL CHEMISTRY, vol.895, 2021 (SCI-Expanded)
- XXVII. **Ammonia Sensing Performance of Polyaniline-Coated Polyamide 6 Nanofibers**  
Pang Z., YILDIRIM E., Pasquinelli M. A., Wei Q.  
ACS OMEGA, vol.6, no.13, pp.8950-8957, 2021 (SCI-Expanded)
- XXVIII. **Altering Electronic and Optical Properties of Novel Benzothiadiazole Comprising Homopolymers via  $\pi$  Bridges**  
Karaman C., Goeker S., Hacıoglu Ş., Hacıfendioglu T., YILDIRIM E., TOPPARE L. K.  
Journal of the Electrochemical Society, vol.168, no.3, 2021 (SCI-Expanded)
- XXIX. **X-ray photoelectron spectroscopy study on the photodegradation of copolyester model compounds**  
Arangdad K., Yildirim E., Detwiler A., Cleven C. D., Burk C., Shamey R., Pasquinelli M. A., Freeman H., El-Shafei A.  
JOURNAL OF APPLIED POLYMER SCIENCE, vol.138, no.2, 2021 (SCI-Expanded)
- XXX. **Construction of amperometric biosensor modified with conducting polymer/carbon dots for the analysis of catechol**  
Yasa M., Deniz A., Forough M., YILDIRIM E., PERSİL ÇETİNKOL Ö., Udum Y. A., TOPPARE L. K.  
Journal of Polymer Science, vol.58, no.23, pp.3336-3348, 2020 (SCI-Expanded)
- XXXI. **Influence of hydrogen bond on the mesomorphic behaviour in urethane based liquid crystalline compounds: Experimental and computer simulation study**  
Korkmaz B., Agtas S., Sutay B., YILDIRIM E., Yilgor I., Yurtsever M., Şenkal B. F., Gürsel Y.  
JOURNAL OF MOLECULAR LIQUIDS, vol.317, 2020 (SCI-Expanded)
- XXXII. **A comprehensive study: Theoretical and experimental investigation of heteroatom and substituent effects on frontier orbitals and polymer solar cell performances**  
Cevher Ş. C., Hizalan G., Alemdar Yilmaz E., Cevher D., Udum Arslan Y., Toppare L., Yıldırım E., Çırpan A.  
JOURNAL OF POLYMER SCIENCE, vol.58, no.19, pp.2792-2806, 2020 (SCI-Expanded)
- XXXIII. **Thermoelectric polymer films with a significantly high Seebeck coefficient and thermoelectric power factor obtained through surface energy filtering**  
Guan X., Yildirim E., Fan Z., Lu W., Li B., Zeng K., Yang S., Ouyang J.  
JOURNAL OF MATERIALS CHEMISTRY A, vol.8, no.27, pp.13600-13609, 2020 (SCI-Expanded)
- XXXIV. **Effect of substituents in sulfoxides on the enhancement of thermoelectric properties of PEDOT:PSS: experimental and modelling evidence**  
Zhu Q., Yildirim E., Wang X., Kyaw A. K. K., Tang T., Soo X. Y. D., Wong Z. M., Wu G., Yang S., Xu J.  
MOLECULAR SYSTEMS DESIGN & ENGINEERING, vol.5, no.5, pp.976-984, 2020 (SCI-Expanded)
- XXXV. **The Role of Electrostatic Interaction between Free Charge Carriers and Counterions in Thermoelectric Power Factor of Conducting Polymers: From Crystalline to Polycrystalline Domains**  
Shi W., Yildirim E., Wu G., Wong Z. M., Deng T., Wang J., Xu J., Yang S.  
ADVANCED THEORY AND SIMULATIONS, vol.3, no.6, 2020 (SCI-Expanded)

- XXXVI. **Correlating charge and thermoelectric transport to paracrystallinity in conducting polymers.**  
Abutaha A., Kumar P., Yildirim E., Shi W., Yang S., Wu G., Hippalgaonkar K.  
Nature communications, vol.11, pp.1737, 2020 (SCI-Expanded)
- XXXVII. **The impact of [1,2,5]chalcogenazolo[3,4-f]-benzo[1,2,3]triazole structure on the optoelectronic properties of conjugated polymers**  
Alkan E. A., GÖKER S., Sarigul H., YILDIRIM E., Udum Y. A., Toppare L.  
JOURNAL OF POLYMER SCIENCE, vol.58, no.7, pp.956-968, 2020 (SCI-Expanded)
- XXXVIII. **Physical Characterization of Inclusion Complexes of Triphenyl Phosphate and Cyclodextrins in Solution.**  
Zhang N., Zane C., Chen Y., Yildirim E., Hinks D., Tonelli A., Vinueza N., Pasquinelli M.  
The journal of physical chemistry. B, vol.124, pp.404-412, 2020 (SCI-Expanded)
- XXXIX. **Improved Alignment of PEDOT:PSS Induced by in-situ Crystallization of "Green" Dimethylsulfone Molecules to Enhance the Polymer Thermoelectric Performance**  
Zhu Q., Yildirim E., Wang X., Soo X. Y. D., Zheng Y., Tan T. L., Wu G., Yang S., Xu J.  
FRONTIERS IN CHEMISTRY, vol.7, 2019 (SCI-Expanded)
- XL. **Proquinoidal-Conjugated Polymer as an Effective Strategy for the Enhancement of Electrical Conductivity and Thermoelectric Properties**  
Tam T. L. D., Ng C. K., Lim S. L., Yildirim E., Ko J., Leong W. L., Yang S., Xu J.  
CHEMISTRY OF MATERIALS, vol.31, no.20, pp.8543-8550, 2019 (SCI-Expanded)
- XLI. **Theoretical design of high-mobility bithiophene imide (BTI) derivative polymeric semiconductors**  
Sutay B., Onaran G., Yildirim E., Yurtsever M.  
COMPUTATIONAL MATERIALS SCIENCE, vol.166, pp.162-169, 2019 (SCI-Expanded)
- XLII. **Influence of UV stabilizers on the weathering of PETG and PCTT films**  
Arangdad K., Yildirim E., Detwiler A., Cleven C. D., Burk C., Shamey R., Pasquinelli M. A., Freeman H. S., El-Shafei A.  
JOURNAL OF APPLIED POLYMER SCIENCE, vol.136, no.47, 2019 (SCI-Expanded)
- XLIII. **Role of Local Polymer Conformations on the Diverging Glass Transition Temperatures and Dynamic Fragilities of Isotactic-, Syndiotactic-, and Atactic-Poly(methyl methacrylate)s**  
Shen J., Yildirim E., Li S., Caydamli Y., Pasquinelli M. A., Tonelli A. E.  
MACROMOLECULES, vol.52, no.10, pp.3897-3908, 2019 (SCI-Expanded)
- XLIV. **Self-Organization of PEDOT:PSS Induced by Green and Water-Soluble Organic Molecules**  
Yidirim E., Zhu Q., Wu G., Tan T. L., Xu J., Yang S.  
JOURNAL OF PHYSICAL CHEMISTRY C, vol.123, no.15, pp.9745-9755, 2019 (SCI-Expanded)
- XLV. **An experimental and computational approach to pH-dependent self-aggregation of poly(2-isopropyl-2-oxazoline)**  
Çağlı E., Yildirim E., Yang S., Erel Göktepe İ.  
JOURNAL OF POLYMER SCIENCE PART B-POLYMER PHYSICS, vol.57, pp.210-221, 2019 (SCI-Expanded)
- XLVI. **Polymer morphology and interfacial charge transfer dominate over energy-dependent scattering in organic-inorganic thermoelectrics**  
Kumar P., Zaia E. W., Yildirim E., Repaka D. V. M., Yang S., Urban J. J., Hippalgaonkar K.  
NATURE COMMUNICATIONS, vol.9, 2018 (SCI-Expanded)
- XLVII. **CoFe2O4 Nanocrystals Mediated Crystallization Strategy for Magnetic Functioned ZSM-5 Catalysts**  
Li B., Yildirim E., Li W., Qi D., Yu J., Wei J., Liu Z., Sun Z., Liu Y., Kong B., et al.  
ADVANCED FUNCTIONAL MATERIALS, vol.28, no.32, 2018 (SCI-Expanded)
- XLVIII. **A theoretical mechanistic study on electrical conductivity enhancement of DMSO treated PEDOT:PSS**  
Yildirim E., Wu G., Yong X., Tan T. L., Zhu Q., Xu J., Ouyang J., Wang J., Yang S.  
JOURNAL OF MATERIALS CHEMISTRY C, vol.6, no.19, pp.5122-5131, 2018 (SCI-Expanded)
- XLIX. **Experimental and MD simulation study on the physical and mechanical properties of organically modified montmorillonite clay and compatibilized linear low density polyethylene nanocomposites**  
Yildirim E., Yurtsever M., Eriman B., Uyanik N.  
JOURNAL OF APPLIED POLYMER SCIENCE, vol.135, no.6, 2018 (SCI-Expanded)
- L. **Nanoscale considerations responsible for diverse macroscopic phase behavior in monosubstituted**

## **isobutyl-POSS/poly(ethylene oxide) blends**

Caydamli Y., Yildirim E., Shen J., Fang X., Pasquinelli M. A., Spontak R. J., Tonelli A. E.  
SOFT MATTER, vol.13, no.46, pp.8672-8677, 2017 (SCI-Expanded)

- L.I. **Structure-property relationships: Influence of number of anchoring groups in triphenylamine-carbazole motifs on light harvesting and photovoltaic performance for dye-sensitized solar cells**  
Elsherbiny D., Yildirim E., El-Essawy F., Abdel-Megied A., El-Shafei A.  
DYES AND PIGMENTS, vol.147, pp.491-504, 2017 (SCI-Expanded)
- L.II. **A comparative study of the influence of N, N '-dialkyl vs. N, N '-diaryl-based electron donor ancillary ligands on photocurrent and photovoltage in dye-sensitized solar cells (DSSCs)**  
Ashraf S., Yildirim E., Akhtar J., Siddiqi H. M., El-Shafei A.  
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, vol.19, no.31, pp.20847-20860, 2017 (SCI-Expanded)
- L.III. **Synthetic Design of Polyester Electrolytes Guided by Hydrophobicity Calculations**  
Yildirim E., Dakshinamoorthy D., Peretic M. J., Pasquinelli M. A., Mathers R. T.  
MACROMOLECULES, vol.49, no.20, pp.7868-7876, 2016 (SCI-Expanded)
- L.IV. **Effect of intersegmental interactions on the morphology of segmented polyurethanes with mixed soft segments: A coarse-grained simulation study**  
Yildirim E., Yurtsever M., Wilkes G. L., Yilgor I.  
POLYMER, vol.90, pp.204-214, 2016 (SCI-Expanded)
- L.V. **Hierarchical multi-component nanofiber separators for lithium polysulfide capture in lithium-sulfur batteries: an experimental and molecular modeling study**  
Zhu J., Yildirim E., Aly K., Shen J., Chen C., Lu Y., Jiang M., Kim D., Tonelli A. E., Pasquinelli M. A., et al.  
JOURNAL OF MATERIALS CHEMISTRY A, vol.4, no.35, pp.13572-13581, 2016 (SCI-Expanded)
- L.VI. **Thermal Transitions in Polyelectrolyte Assemblies Occur via a Dehydration Mechanism**  
Yildirim E., Zhang Y., Lutkenhaus J. L., Sammalkorpi M.  
ACS MACRO LETTERS, vol.4, no.9, pp.1017-1021, 2015 (SCI-Expanded)
- L.VII. **The influence of ionic strength and mixing ratio on the colloidal stability of PDAC/PSS polyelectrolyte complexes**  
Zhang Y., Yildirim E., Antila H. S., Valenzuela L. D., Sammalkorpi M., Lutkenhaus J. L.  
SOFT MATTER, vol.11, no.37, pp.7392-7401, 2015 (SCI-Expanded)
- L.VIII. **Understanding the influence of hydrogen bonding and diisocyanate symmetry on the morphology and properties of segmented polyurethanes and polyureas: Computational and experimental study**  
Sami S., Yildirim E., Yurtsever M., Yurtsever E., Yilgor E., Yilgor I., Wilkes G. L.  
POLYMER, vol.55, no.18, pp.4563-4576, 2014 (SCI-Expanded)
- L.IX. **The role of diisocyanate and soft segment on the intersegmental interactions in urethane and urea based segmented copolymers: A DFT study**  
Yildirim E., Yurtsever M.  
COMPUTATIONAL AND THEORETICAL CHEMISTRY, vol.1035, pp.28-38, 2014 (SCI-Expanded)
- L.X. **Theoretical approach to the structural, electronic, and morphological properties of poly(E >-caprolactone) grafted polypyrroles**  
Yildirim E., Erciyas G., Yurtsever M.  
MACROMOLECULAR RESEARCH, vol.21, no.9, pp.949-957, 2013 (SCI-Expanded)
- L.XI. **MORPHOLOGICAL PROPERTIES OF PYRROLE AND PHENYLENE ROD-COIL DIBLOCK COPOLYMERS BY DISSIPATIVE PARTICLE DYNAMICS**  
Yildirim E., Yurtsever M.  
JOURNAL OF THEORETICAL & COMPUTATIONAL CHEMISTRY, vol.12, no.1, 2013 (SCI-Expanded)
- L.XII. **Silver-Sodium Ion Exchange Dynamics in LTA Zeolite Membranes**  
Salmas R. E., Demir B., Yildirim E., Sirkecioğlu A., Yurtsever M., Ahunbay M. G.  
JOURNAL OF PHYSICAL CHEMISTRY C, vol.117, no.4, pp.1663-1671, 2013 (SCI-Expanded)
- L.XIII. **Multiscale Modeling of the Morphology and Properties of Segmented Silicone-Urea Copolymers**  
Yildirim E., Yurtsever M., Yurtsever E., Yilgor I., Yilgor E.  
JOURNAL OF INORGANIC AND ORGANOMETALLIC POLYMERS AND MATERIALS, vol.22, no.3, pp.604-616, 2012

(SCI-Expanded)

- LXIV. **A comparative study on the efficiencies of polyethylene compatibilizers by using theoretical methods**  
Yildirim E., Yurtsever M.  
JOURNAL OF POLYMER RESEARCH, vol.19, no.2, 2012 (SCI-Expanded)
- LXV. **Microphase Separation of Phenylene Oligomers with Polymeric Side Chains: A Dissipative Particle Dynamics Study**  
Yildirim E., Yurtsever M., Kenarli B., Demirel A. L.  
MACROMOLECULAR THEORY AND SIMULATIONS, vol.20, no.5, pp.340-349, 2011 (SCI-Expanded)
- LXVI. **A QSPR Study on the Physical Properties of Substituted Polypyrroles and Poly(paraphenylenes)**  
Yildirim E., Aksoy D., Tuzun N. S., Yurtsever M.  
DESIGNED MONOMERS AND POLYMERS, vol.14, no.1, pp.79-93, 2011 (SCI-Expanded)
- LXVII. **Solvation of K<sup>+</sup> in helium droplets**  
Yurtsever E., Yildirim E., Yurtsever M., Bodo E., Gianturco F. A.  
EUROPEAN PHYSICAL JOURNAL D, vol.43, pp.105-108, 2007 (SCI-Expanded)
- LXVIII. **Bosonic helium clusters doped by alkali metal cations: interaction forces and analysis of their most stable structures**  
Marinetti F., Coccia E., Bodo E., Gianturco F. A., Yurtsever E., Yurtsever M., Yildirim E.  
THEORETICAL CHEMISTRY ACCOUNTS, vol.118, no.1, pp.53-65, 2007 (SCI-Expanded)
- LXIX. **Bosonic helium droplets with cationic impurities: Onset of electrostriction and snowball effects from quantum calculations**  
Coccia E., Bodo E., Marinetti F., Gianturco F. A., Yildirim E., Yurtsever M., Yurtsever E.  
JOURNAL OF CHEMICAL PHYSICS, vol.126, no.12, 2007 (SCI-Expanded)

## Articles Published in Other Journals

- I. **Improved Eco-Friendliness of a Common Flame Retardant through Inclusion Complexation with Cyclodextrins**  
Zhang N., Yildirim E., Zane C. P., Shen J., Vinueza N., Hinks D., Tonelli A. E., Pasquinelli M. A.  
ACS APPLIED POLYMER MATERIALS, vol.1, no.10, pp.2768-2777, 2019 (ESCI)

## Refereed Congress / Symposium Publications in Proceedings

- I. **MECHANISM OF AGGREGATION CONTROL BY DETERGENT AND DISPERSANTS: A MULTISCALE MODELING STUDY**  
Özdemir E., Kan E., Guo B., Ağiral A., Yıldırım E.  
CPC XIII 13th Chemical Physics Congress, Elazığ, Turkey, 07 October 2022 - 08 January 2023, pp.27
- II. **Electrical Conductivity Enhancement Mechanism of Acid Treated PEDOT:PSS by Molecular Modeling Methods**  
Özdemir E., Yıldırım E.  
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## **Metrics**

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