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Education Information

Doctorate, Cornell University, Turkey 1999 - 2005
Undergraduate, Middle East Technical University, Faculty of Arts and Sciences, Department of Physics, Turkey 1995 - 1999

Dissertations

Doctorate, Quantitative Prediction of Elastic and Anelastic Phenomena on the Nanometer Scale ?, Cornell University, 2005

Research Areas

Natural Sciences

Academic Titles / Tasks

Associate Professor, Middle East Technical University, Faculty of Arts and Sciences, Department of Physics, 2017 - Continues
Assistant Professor, Middle East Technical University, Faculty of Arts and Sciences, Department of Physics, 2007 - 2017

Advising Theses

TOFFOLİ H., Molecular dynamics modelling of gold atomic force microscopy tips on multilayer graphene, Postgraduate, C.Maden(Student), 2020
TOFFOLİ H., Theoretical investigation of the nanotribological properties of the hexagonal boron nitride and gold interfaces, Postgraduate, G.Özcan(Student), 2020
TOFFOLİ H., A joint density functional and classical molecular dynamics study on interface characteristics of graphene and polyetheretherketone, Postgraduate, E.Sert(Student), 2020

TOFFOLİ H., AB initio investigation of the nanotribological properties of MoS2/Au(111) interface, Postgraduate, Ü.Doğan(Student), 2020
TOFFOLİ H., Tight binding investigation of graphene nanostructures under magnetic field, Postgraduate, F.YALÇIN(Student), 2019
TOFFOLİ H., AB initio investigation of the nanotribological properties of the h-BN/h-BN and the h-BN/Au(111) interfaces, Postgraduate, M.Baksi(Student), 2019
TOFFOLİ H., A Density functional theory investigation for solid state hydrogen storage materials, Doctorate, A.Gencer(Student), 2018
GÜRSES E., TOFFOLİ H., Density functional theory and molecular dynamics simulations of carbon nanotubes, polyetheretherketone and their interfaces, Postgraduate, G.TORAMAN(Student), 2018
TOFFOLİ H., Density functional theory investigation on thickness and load dependency of friction force between graphene and Au interfaces, Postgraduate, D.GİZEM(Student), 2018
TOFFOLİ H., Atomistic insights into surface reactivity via density functional theory, Doctorate, M.DEMİRTAŞ(Student), 2018
TOFFOLİ H., Ab initio modelling of materials properties for catalytic and device applications, Doctorate, M.GÖKHAN(Student), 2017
TOFFOLİ H., AKATA KURÇ B., Covalent and non-covalent functionalization of graphene for application in catalysis and device technology: A first principles computational study, Doctorate, T.İRFAN(Student), 2017
TOFFOLİ H., Density functional theory investigation of the reaction mechanisms for selective oxidation of alcohols on gold catalysts, Postgraduate, O.DERNEK(Student), 2016
MEHRABOV A., TOFFOLİ H., Synthesis and structural characterization of Ni-B nanoalloys, Postgraduate, L.Seda(Student), 2015
TOFFOLİ H., A density functional theory investigation of graphene-based materials, Doctorate, C.SİBEL(Student), 2014
TOFFOLİ H., Density functional theory investigation of dipolar ultracold atoms in harmonic traps, Postgraduate, O.KARACA(Student), 2014
TOFFOLİ H., Investigation of catalytic properties and electronic structure of correlated material CeO2 with ab-initio computational methods, Postgraduate, B.ÖZDEMİR(Student), 2013
AKATA KURÇ B., TOFFOLİ H., Modelling and experimental study of titanosilicate ETS-10: application for solar cells, Postgraduate, M.KOÇ(Student), 2013
TOFFOLİ H., Örgü sabitleri uyusmayan III-V yarıiletken nanotellerinin elektronik ve geometrik özelliklerinin yoğunluk fonksiyonel teorisi ile incelenmesi, Doctorate, B.ÖZKAPI(Student), 2012
TOFFOLİ H., Molecular dynamics investigation of moire patterns in double-layer graphene, Postgraduate, G.SÖKMEN(Student), 2012
TOFFOLİ H., The effects of promoters on the sulfur resistance of NOx storage/reduction catalysts: A density functional theory investigation, Postgraduate, R.KOŞAK(Student), 2011
TOFFOLİ H., Density functional theory investigation of noble metal reduction agents on ?-aluminum oxide in NOx storage/reduction catalysts, Postgraduate, Z.ARTUÇ(Student), 2011
TOFFOLI D., TOFFOLİ H., Density functional theory investigation of noble metal reduction agents on Gamma-Al2O3 in NOx storage/reduction catalysis /, Postgraduate, Z.Artuç(Student), 2011
TOFFOLİ H., Effect of support material in NOx storage/reduction catalysts, Postgraduate, R.HUMMATOV(Student), 2010
TOFFOLİ H., Density functional theory investigation of TiO2 anatase nanosheets, Postgraduate, C.SİBEL(Student), 2009
TOFFOLİ H., Density functional theory for trapped ultracold fermions, Postgraduate, Ö.AKYAR(Student), 2009
TOFFOLİ H., Electronic properties of dye molecules adsorbed on anatase-titania surface for solar cell applications, Postgraduate, E.TORUN(Student), 2009

Published journal articles indexed by SCI, SSCI, and AHCI

I. **Development of a selective wet-chemical etchant for precise 3D sculpting of silicon enabled by infrared non-linear laser modification**
   Zolfaghari Borra M., Radfar B., Nasser H., Çolakoğlu T., Tokel O., Turnalı A., DEMİRTAŞ M., Işık Taşgın D., TOFFOLİ

H., Toffoli D., et al.
Optics and Laser Technology, vol.176, 2024 (SCI-Expanded)

II. **Oxygen-Promoted on-Surface Synthesis of Polyboroxine Molecules**
Toffoli D., Turco E., Stredansky M., Costantini R., Dell'Angela M., Floreano L., Goldoni A., Morgante A., Kladnik G., Cvetko D., et al.
Chemistry - A European Journal, vol.30, no.47, 2024 (SCI-Expanded)

III. **Insights into Reaction Mechanisms in Liquid Metals from Density Functional Theory: CH4 Pyrolysis in BiNiX (X = Cu, Al) Molten Metals as a Case Study**
Erbasan A., TOFFOLİ H., Toffoli D., GÖKALP İ., KARDAŞ G., ÇELİK G.
ACS Applied Energy Materials, vol.7, no.8, pp.3220-3233, 2024 (SCI-Expanded)

IV. **A Classical Molecular Dynamics Study of the Effect of the Atomic Force Microscope Tip Shape, Size and Deformation on the Tribological Properties of the Graphene/Au(111) Interface**
Maden C., TOFFOLİ H., Toffoli D.
Lubricants, vol.12, no.2, 2024 (SCI-Expanded)

V. **Hydrogen production using aluminum-water splitting: A combined experimental and theoretical approach**
Kandasamy J., Mutlu R. N., Eroğlu E., KARACA M., TOFFOLİ H., GÖKALP İ.
International Journal of Hydrogen Energy, vol.52, pp.202-211, 2024 (SCI-Expanded)

VI. **Effect of Surface Pt Doping on the Reactivity of Au(111) Surfaces towards Methanol Dehydrogenation: A First-Principles Density Functional Theory Investigation**
Demirtas M., TOFFOLİ H., Toffoli D.
Molecules, vol.28, no.23, 2023 (SCI-Expanded)

VII. **Temperature-dependent thermoelastic properties of GaSb and InSb semiconductors: Identification through ab initio DFT simulations**
Baloğlu E. C., TOFFOLİ H., DAL H.
Physica B: Condensed Matter, vol.643, 2022 (SCI-Expanded)

VIII. **Formaldehyde Selectivity in Methanol Partial Oxidation on Silver: Effect of Reactive Oxygen Species, Surface Reconstruction, and Stability of Intermediates**
Karatok M., ŞENSOY M. G., Vovk E. I., TOFFOLİ H., Toffoli D., Ozensoy E.
ACS Catalysis, vol.11, no.10, pp.6200-6209, 2021 (SCI-Expanded)

IX. **Polymer interfaces with carbon nanostructures: First principles density functional theory and molecular dynamics study of polyetheretherketone adsorption on graphene and nanotubes**
Toraman G., Sert E., Gulasik H., Toffoli D., TOFFOLİ H., GÜRSES E.
COMPUTATIONAL MATERIALS SCIENCE, vol.191, 2021 (SCI-Expanded)

X. **Methylamine terminated molecules on Ni(111): A path to low temperature synthesis of nitrogen-doped graphene**
Costantini R., TOFFOLİ H., Feng Z., Stredansky M., Toffoli D., Fronzoni G., Dri C., Comelli G., Cvetko D., Kladnik G., et al.
FLATCHEM, vol.24, 2020 (SCI-Expanded)

XI. **First-principles investigation of CO and CO2 adsorption on gamma-Al2O3 supported monoatomic and diatomic Pt clusters**
Sensoy M. G., Ustunel H., Toffoli D.
APPLIED SURFACE SCIENCE, vol.499, 2020 (SCI-Expanded)

XII. **Nanotribological Properties of the h-BN/Au(111) Interface: A DFT Study**
Baksi M., Toffoli D., GÜLSEREN O., Ustunel H.
JOURNAL OF PHYSICAL CHEMISTRY C, vol.123, no.46, pp.28411-28418, 2019 (SCI-Expanded)

XIII. **Combined effect of point defects and layer number on the adsorption of benzene and toluene on graphene**
Akay T. I., Toffoli D., TOFFOLİ H.
APPLIED SURFACE SCIENCE, vol.480, pp.1063-1069, 2019 (SCI-Expanded)

XIV. **Instability of a Noncrystalline NaO2 Film in Na-O-2 Batteries: The Controversial Effect of the RuO2**

Catalyst
Tovini M. F., Hong M., Park J., Demirtas M., Toffoli D., Ustunel H., Byon H. R., YILMAZ E.
JOURNAL OF PHYSICAL CHEMISTRY C, vol.122, no.34, pp.19678-19686, 2018 (SCI-Expanded)

XV. **Effect of Platinum, Gold, and Potassium Additives on the Surface Chemistry of CdI2-Antitype Mo2C**
Dernirtas M., Ustunel H., Toffoli D.
ACS OMEGA, vol.2, no.11, pp.7976-7984, 2017 (SCI-Expanded)

XVI. **Comparative Analysis of Reactant and Product Adsorption Energies in the Selective Oxidative Coupling of Alcohols to Esters on Au(111)**
Senozan S., TOFFOLİ H., Karatok M., Vovk E. I., Shah A. A., ÖZENSOY E., Toffoli D.
TOPICS IN CATALYSIS, vol.59, pp.1383-1393, 2016 (SCI-Expanded)

XVII. **Multiscale Self-Assembly of Silicon Quantum Dots into an Anisotropic Three-Dimensional Random Network**
İlday S. K., İlday F. Ö., Huebner R., Prosa T. J., Martin I., Nogay G., Kabacelik I., Mics Z., Bonn M., Turchinovich D., et al.
NANO LETTERS, vol.16, pp.1942-1948, 2016 (SCI-Expanded)

XVIII. **Active role of the support in NOx storage and reductioncatalytic systems**
Tek M., TOFFOLİ H., Toffoli D.
APPLIED SURFACE SCIENCE, vol.355, pp.1295-1305, 2015 (SCI-Expanded)

XIX. **Covalent and noncovalent functionalization of pristine and defective graphene by cyclohexane and dehydrogenated derivatives**
Sayin C. S., Toffoli D., TOFFOLİ H.
APPLIED SURFACE SCIENCE, vol.351, pp.344-352, 2015 (SCI-Expanded)

XX. **Understanding the Effects of Ion-Exchange in Titanosilicate ETS-10: A Joint Theoretical and Experimental Study**
Koc M., Galioglu S., Toffoli D., TOFFOLİ H., AKATA KURÇ B.
JOURNAL OF PHYSICAL CHEMISTRY C, vol.118, no.47, pp.27281-27291, 2014 (SCI-Expanded)

XXI. **Bis(triisopropylsilylethynyl)pentacene/Au(111) Interface: Coupling, Molecular Orientation, and Thermal Stability**
Gnoli A., Ustunel H., TOFFOLI D., Yu L., Catone D., Turchini S., Lizzit S., Stingelin N., Larciprete R.
JOURNAL OF PHYSICAL CHEMISTRY C, vol.118, no.39, pp.22522-22532, 2014 (SCI-Expanded)

XXII. **Insights into surface-adsorbate interactions in corrosion inhibition processes at the molecular level**
ÖZCAN M., Toffoli D., Ustunel H., DEHRİ İ.
CORROSION SCIENCE, vol.80, pp.482-486, 2014 (SCI-Expanded)

XXIII. **First principles investigation of NO2 and SO2 adsorption on gamma-Al2O3 supported mono- and diatomic metal clusters**
Artuc Z., Ustunel H., Toffoli D.
RSC ADVANCES, vol.4, no.89, pp.48492-48506, 2014 (SCI-Expanded)

XXIV. **First-Principles Investigation of NOx and SOx Adsorption on Anatase-Supported BaO and Pt Overlayers**
Hummatov R., GÜLSEREN O., ÖZENSOY E., Toffoli D., TOFFOLİ H.
JOURNAL OF PHYSICAL CHEMISTRY C, vol.116, no.10, pp.6191-6199, 2012 (SCI-Expanded)

XXV. **Metallization of the C-60/Rh(100) interface revealed by valence photoelectron spectroscopy and density functional theory calculations**
Wade A., Lizzit S., Petaccia L., Goldoni A., Diop D., Ustunel H., Fabris S., Baroni S.
JOURNAL OF CHEMICAL PHYSICS, vol.132, no.23, 2010 (SCI-Expanded)

XXVI. **The self-consistent calculation of exchange enhanced odd integer quantized Hall plateaus within Thomas-Fermi-Dirac approximation**
Bilgec G., TOFFOLİ H., Siddiki A., SÖKMEN İ.
PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES, vol.42, no.4, pp.1058-1061, 2010 (SCI-Expanded)

XXVII. **Structural, Electronic and Magnetic Properties of BN Nanotubes Doped with Mn and Cr: Exploring the Potential for Device Technology**
KÖKTEN H., Ustunel H., ERKOÇ Ş.

JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, vol.6, no.4, pp.926-932, 2009 (SCI-Expanded)

XXVIII. **High-capacity hydrogen storage by metallized graphene**
Ataca C., Akturk E., ÇIRACI S., Ustunel H.
APPLIED PHYSICS LETTERS, vol.93, no.4, 2008 (SCI-Expanded)

XXIX. **Structural properties and stability of nanoclusters**
Ustuenel H., Erkoc S.
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, vol.4, no.5, pp.928-956, 2007 (SCI-Expanded)

XXX. **Defect-controlled transport properties of metallic atoms along carbon nanotube surfaces**
Barinov A., Uestuenel H., Fabris S., Gregoratti L., Aballe L., Dudin P., Baroni S., Kiskinova M.
PHYSICAL REVIEW LETTERS, vol.99, no.4, 2007 (SCI-Expanded)

XXXI. **Modeling a suspended nanotube oscillator**
Ustunel H., Roundy D., Arias T.
NANO LETTERS, vol.5, no.3, pp.523-526, 2005 (SCI-Expanded)

XXXII. **Ab initio mechanical response: Internal friction and structure of divacancies in silicon**
Ustunel H., Roundy D., Arias T.
PHYSICAL REVIEW LETTERS, vol.94, no.2, 2005 (SCI-Expanded)

XXXIII. **A tunable carbon nanotube electromechanical oscillator**
Sazonova V., Yaish Y., Ustunel H., Roundy D., Arias T., McEuen P.
NATURE, vol.431, no.7006, pp.284-287, 2004 (SCI-Expanded)

XXXIV. **Electron-phonon scattering in metallic single-walled carbon nanotubes**
Park J., Rosenblatt S., Yaish Y., Sazonova V., Ustunel H., Braig S., Arias T., Brouwer P., McEuen P.
NANO LETTERS, vol.4, no.3, pp.517-520, 2004 (SCI-Expanded)

Articles Published in Other Journals

I. **Tribology at the atomic scale with density functional theory**
TOFFOLİ H., Toffoli D.
Electronic Structure, vol.4, no.2, 2022 (ESCI)

Refereed Congress / Symposium Publications in Proceedings

I. **NiX (X: Al, Bi, Cu, Ga, In, Sn, Zn, Zr) İkili Metal Alaşımları Kullanılarak Metan Gazından H2 Gazı Eldesinin DFT Metodu ile İncelenmesi**
Eroğlu E., TOFFOLİ H., Erbasan A., Tosun S. M., Öğrence Ç., Sökmen U., Mutlu R. N., KARDAŞ G., Gökalp İ., ÇELİK G.
Yoğun Madde Fiziği (YMF28) – Ankara Toplantısı, Ankara, Turkey, 22 December 2023

II. **Düzensiz Ortamlarda Reaksiyon Dinamiği Teorisi: BiNiX Üçlü Metal Alaşımları Kullanılarak CH4 gazından H2 eldesi**
TOFFOLİ H., Erbasan A., Sökmen U., Eroğlu E., Mutlu R. N., KARDAŞ G., Gökalp İ., ÇELİK G.
X. Yoğun Madde Fiziği - İzmir Toplantısı, İzmir, Turkey, 28 April 2023

III. **Altın ve Grafen Yüzeyleri Arasındaki Etkileşimin Yük Yoğunluğu Fonksiyoneli Teorisi Kullanılarak İncelenmesi**
Şentürk D. G., TOFFOLİ H.
Yoğun Madde Fiziği, Turkey, 22 December 2017

IV. **Ethanol dehydrogenation on the Ni-and Rh-doped Au(111) surface**
Dernek O., TOFFOLİ H.
Yoğun Madde Fiziği, Turkey, 22 December 2017

V. **A comparative study of the polymer-nanotube interface through a reactive force field and density functional theory**
Toffoli H., Gürses E., Gülaşık H., Konuk M., Sert E., Toraman G.

International Symposium on Chemistry via Computation, Ankara, Turkey, 30 October 2017

VI. **Molecular Dynamics Simulations of Carbon Nanotube Reinforced Polymer Composites**
Toraman G., Konuk M., Sert E., Toffoli H., Gülaşık H., Gürses E.
9th Ankara International Aerospace Conference, Ankara, Turkey, 20 - 22 September 2017

VII. **Multi-Scale Modelling of Carbon Nanotube Reinforced Polymer Composites**
Toraman G., Konuk M., Gülaşık H., Sert E., Toffoli H., Gürses E.
Materials Resistant to Extreme Conditions for Future Energy Systems, Kyyiv, Ukraine, 12 - 14 June 2017

VIII. **Alkollerin Seçici Oksidasyonu için Nümerik Malzeme Bilimiile Katalizör Tasarımı**
TOFFOLİ H.
Yoğun Madde Fiziği Toplantısı, Turkey, 16 December 2016

IX. **Density functional theory Investigation of the Ni and RhdopedAu 111 surface as a viable catalyst for selective oxidation ofethanol**
Dernek O., Toffoli D., TOFFOLİ H.
Nano2016, 7 - 12 August 2016

X. **Application of density functional theory methods to two dimensional harmonically confined dipolar atoms**
TOFFOLİ H.
İstanbul Teknik Üniversitesi, 23 - 14 June 2016

XI. **Performance of Mo2C as a catalyst for the water gas shift reaction a DFT investigation**
Toffoli D., DEMİRTAŞ M., ÜSTÜNEL H.
Nano TR 11 Ankara 2015, Ankara, Turkey, 22 - 25 June 2015

XII. **Active Role of the Support in NOx Storage and Reduction Systems**
TEK M., Toffoli D., Üstünel H.
NanoTR 11, 22 - 23 June 2015

XIII. **Methanol Dehydrogenation on bare and atomic oxygen pre covered Au 111 and Ag doped Au 111 surfaces**
Selma Ş., Üstünel H., Toffoli D.
NanoTR11, 22 - 26 June 2015

XIV. **Density Functional Theory Investigation of the Structural Electronic and Adsorption Properties of 100 110 111 surfaces of Zincblende PtC**
ŞENSOY M. G., Üstünel H., Toffoli D.
NanoTR 11, 22 - 25 June 2015

XV. **Density functional theory investigation of two-dimensional dipolar fermions in a harmonic trap**
TOFFOLİ H., Abedinpour S. H., TANATAR B.
27th International Conference on Low Temperature Physics (LT), Buenos Aires, Argentina, 6 - 13 August 2014, vol.568

XVI. **HEGZAGONAL BN/AU(111) YÜZEYLERI ARASINDAKI NANOTRIBOLOJIK ÖZELLIKLERIN AB INITIO HESAPLAR ILE INCELENMESI**
Baksi M., GÜLSEREN O., TOFFOLİ H.
Yoğun Madde Fiziği 23, Turkey, 22 December 2017

XVII. **Kataliz ve Cihaz Teknolojisinde Kullanılmak Üzere Grafenin KovalentOlmayan Şekilde İşlevselleştirilmesi için YFT Çalışması**
Akay T. İ., TOFFOLİ H., Toffoli D.
Yoğun Madde Fiziği 23, Turkey, 22 December 2017

Supported Projects

Toffoli H., Günel Kiliç B., Akagündüz E., Akbaş E., Dülger Ö., Karaca M., Karagöz P., Manguoğlu M., Nazirzadeh S., Sezer Uzol N., et al., EU Supported Other Project, EuroCC2 - National Competence Centers in the Framework of EuroHPC Phase2, 2023 - 2026

Yildirim E., Özkanakti M. H., Erol F., Toffoli H., H2020 Project, Improvement of the Graphene-Epoxy Mixing Recipes for Composites Industry by Understanding Interaction Mechanisms through HPC Calculations (EPOGRAHPC), 2022 - 2023
Ortakaya B., Temizsoylu O., Toffoli H., Yerli S. K., Kaya K., Baran Ö. U., Karaca M., Karagöz P., Koku H., Manguoğlu M., et al., H2020 Project, EuroCC@Türkiye, 2020 - 2022
TOFFOLİ H., TUBITAK Project, İki Boyutlu Sistemler ile Au Arayüzlerinin Nanotribolojik Özellikleri Üzerine Teorik ve Deneysel Bir Çalışma, 2016 - 2019
TOFFOLİ H., NATO Supported Research Project, Advanced Microwave Sources, 2017 - 2018
TOFFOLİ H., TUBITAK Project, Fotoiyonizasyonda Çok ElektronluSüreçlerin Teorik Olarak İncelenmesi, 2016 - 2016
TOFFOLİ H., TUBITAK Project, Altın Katalizörler Üzerinde Alkollerin Seçici Oksitlenmesi Reaksiyon Mekanizmalarının Yük Yoğunluğu Fonksiyoneli Teorisi Ile Incelenmesi, 2013 - 2016
TOFFOLİ H., DEMİRTAŞ M., Project Supported by Higher Education Institutions, SU-GAZ DEĞİŞİMİ MEKANİZMASININ YÜK YOĞUNLUĞU FONKSİYONELİ TEORİSİYLE İNCELENMESİ, 2013 - 2013
TOFFOLİ H., ŞENSOY M. G., Project Supported by Higher Education Institutions, SU-GAZ DEĞİŞİMİ REAKSİYONUNDA ALTTAŞ MALZEMENİN ETKİSİNİN YÜK YOĞUNLUĞU FONKSİYONELİ KULLANILARAK İNCELENMESİ, 2013 - 2013
TOFFOLİ H., TUBITAK Project, Yoğunluk Fonksiyoneli Teorisine Dayanan Temel Prensip Hesabı Ile Pt/Bao/Al2o3 Nox Indirgeme/Depolama Katalizörünün Işleme Mekanizmasının Incelenmesi Ve Verimlileştirilmesi, 2009 - 2012
TOFFOLİ H., Project Supported by Higher Education Institutions, Yarıiletken Nanotellerin Manyetik Atomlarla Katkılandırılması Konusunda Yük Yoğunluğu Fonksiyoneli Hesapları, 2009 - 2009

Metrics

Publication: 59
Citation (WoS): 2532
Citation (Scopus): 2647
H-Index (WoS): 11
H-Index (Scopus): 11

Non Academic Experience

METU
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SISSA
Cornell University