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Publons / Web Of Science ResearcherID: A-3579-2016

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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

Supervised Theses

TOFFOLÌ H., Molecular dynamics modelling of gold atomic force microscopy tips on multilayer graphene, Postgraduate, C.Maden(Student), 2020

TOFFOLÌ H., Theoretical investigation of the nanotribological properties of the hexagonal boron nitride and gold interfaces, Postgraduate, G.Özcan(Student), 2020

TOFFOLÌ H., A joint density functional and classical molecular dynamics study on interface characteristics of graphene and polyetheretherketone, Postgraduate, E.Sert(Student), 2020

TOFFOLÍ H., AB initio investigation of the nanotribological properties of MoS₂/Au(111) interface, Postgraduate, Ü.Doğan(Student), 2020

TOFFOLÍ H., Tight binding investigation of graphene nanostructures under magnetic field, Postgraduate, F.YALÇIN(Student), 2019

TOFFOLÍ 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

TOFFOLÍ H., A Density functional theory investigation for solid state hydrogen storage materials, Doctorate, A.Gencer(Student), 2018

GÜRSES E., TOFFOLÍ H., Density functional theory and molecular dynamics simulations of carbon nanotubes, polyetheretherketone and their interfaces, Postgraduate, G.TORAMAN(Student), 2018

TOFFOLÍ H., Density functional theory investigation on thickness and load dependency of friction force between graphene and Au interfaces, Postgraduate, D.GİZEM(Student), 2018

TOFFOLÍ H., Atomistic insights into surface reactivity via density functional theory, Doctorate, M.DEMİRTAŞ(Student), 2018

TOFFOLÍ H., Ab initio modelling of materials properties for catalytic and device applications, Doctorate, M.GÖKHAN(Student), 2017

TOFFOLÍ 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

TOFFOLÍ H., Density functional theory investigation of the reaction mechanisms for selective oxidation of alcohols on gold catalysts, Postgraduate, O.DERNEK(Student), 2016

MEHRABOV A., TOFFOLÍ H., Synthesis and structural characterization of Ni-B nanoalloys, Postgraduate, L.Seda(Student), 2015

TOFFOLÍ H., A density functional theory investigation of graphene-based materials, Doctorate, C.SİBEL(Student), 2014

TOFFOLÍ H., Density functional theory investigation of dipolar ultracold atoms in harmonic traps, Postgraduate, O.KARACA(Student), 2014

TOFFOLÍ 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., TOFFOLÍ H., Modelling and experimental study of titanosilicate ETS-10: application for solar cells, Postgraduate, M.KOÇ(Student), 2013

TOFFOLÍ H., Örgü sabitleri uyusmayan III-V yarıiletken nanotellerinin elektronik ve geometrik özelliklerinin yoğunluk fonksiyonel teorisi ile incelenmesi, Doctorate, B.ÖZKAPI(Student), 2012

TOFFOLÍ H., Molecular dynamics investigation of moire patterns in double-layer graphene, Postgraduate, G.SÖKMEN(Student), 2012

TOFFOLÍ H., The effects of promoters on the sulfur resistance of NO_x storage/reduction catalysts: A density functional theory investigation, Postgraduate, R.KOŞAK(Student), 2011

TOFFOLÍ H., Density functional theory investigation of noble metal reduction agents on γ -aluminum oxide in NO_x storage/reduction catalysts, Postgraduate, Z.ARTUÇ(Student), 2011

TOFFOLI D., TOFFOLÍ H., Density functional theory investigation of noble metal reduction agents on Gamma-Al₂O₃ in NO_x storage/reduction catalysis /, Postgraduate, Z.Arduç(Student), 2011

TOFFOLÍ H., Effect of support material in NO_x storage/reduction catalysts, Postgraduate, R.HUMMATOV(Student), 2010

TOFFOLÍ H., Density functional theory investigation of TiO₂ anatase nanosheets, Postgraduate, C.SİBEL(Student), 2009

TOFFOLÍ H., Density functional theory for trapped ultracold fermions, Postgraduate, Ö.AKYAR(Student), 2009

TOFFOLÍ 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., TOFFOLÍ

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., TOFFOLI 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., TOFFOLI 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., TOFFOLI 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., TOFFOLI 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., TOFFOLI 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., TOFFOLI 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., TOFFOLI 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., TOFFOLI 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., TOFFOLI H.
APPLIED SURFACE SCIENCE, vol.480, pp.1063-1069, 2019 (SCI-Expanded)
- XIV. **Instability of a Noncrystalline NaO₂ Film in Na-O₂ 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**
Demirtas 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., TOFFOLI 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 NO_x storage and reduction catalytic systems**
Tek M., TOFFOLI 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., TOFFOLI 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., TOFFOLI 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 NO_x and SO_x Adsorption on Anatase-Supported BaO and Pt Overlayers**
Hummatov R., GÜLSEREN O., ÖZENSOY E., Toffoli D., TOFFOLI 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., TOFFOLI 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**
Ustunel H., Erkoç 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., Ustunel 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**
TOFFOLÌ 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) İki Metal Alařımları Kullanılarak Metan Gazından H₂ Gazı Eldesinin DFT Metodu ile İncelenmesi**
Erođlu E., TOFFOLÌ H., Erbasan A., Tosun S. M., Öđrence Ç., Sökmen U., Mutlu R. N., KARDAŞ G., Gökalp İ., ÇELİK G.
Yođun Madde Fiziđi (YMF28) – Ankara Toplantısı, Ankara, Turkey, 22 December 2023
- II. **Düzensiz Ortamlarda Reaksiyon Dinamiđi Teorisi: BiNiX Üçlü Metal Alařımları Kullanılarak CH₄ gazından H₂ eldesi**
TOFFOLÌ H., Erbasan A., Sökmen U., Erođlu E., Mutlu R. N., KARDAŞ G., Gökalp İ., ÇELİK G.
X. Yođun Madde Fiziđi - İzmir Toplantısı, İzmir, Turkey, 28 April 2023
- III. **Altın ve Grafen Yüzeyleri Arasındaki Etkileřimin Yük Yođunluđu Fonksiyoneli Teorisi Kullanılarak İncelenmesi**
Şentürk D. G., TOFFOLÌ H.
Yođun Madde Fiziđi, Turkey, 22 December 2017
- IV. **Ethanol dehydrogenation on the Ni-and Rh-doped Au(111) surface**
Dernek O., TOFFOLÌ H.
Yođun Madde Fiziđi, 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., Gülařık 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, Kyiv, Ukraine, 12 - 14 June 2017
- VIII. **Alkollerin Seçici Oksidasyonu için Nümerik Malzeme Bilimi ile Katalizör Tasarımı**
TOFFOLİ H.
Yoğun Madde Fiziği Toplantısı, Turkey, 16 December 2016
- IX. **Density functional theory Investigation of the Ni and Rh doped Au 111 surface as a viable catalyst for selective oxidation of ethanol**
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 NO_x 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. **HEZAGONAL BN/AU(111) YÜZEYLERİ ARASINDAKİ NANOTRİBOLOJİK ÖZELLİKLERİN AB INITIO HESAPLAR İLE İNCELENMESİ**
Baksi M., GÜLSEREN O., TOFFOLİ H.
Yoğun Madde Fiziği 23, Turkey, 22 December 2017
- XVII. **Kataliz ve Cihaz Teknolojisinde Kullanılmak Üzere Grafenin Kovalent Olmayan Şekilde İşlevselleştirilmesi için YFT Çalışması**
Akay T. İ., TOFFOLİ H., Toffoli D.
Yoğun Madde Fiziği 23, Turkey, 22 December 2017

Metrics

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H-Index (Scopus): 11

Non Academic Experience

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Cornell University