

Assoc. Prof. HANDE TOFFOLÌ

Personal Information

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Education Information

Doctorate, Cornell University, Turkey 1999 - 2005

Under Graduate, 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

Advising Theses

TOFFOLÌ H., Tight binding investigation of graphene nanostructures under magnetic field, Post Graduate, F.YALÇIN(Student), 2019

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

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

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

AKATA KURÇ B., TOFFOLÌ H., Covalent and non-covalent functionalization of graphene for application in catalysis and device technology: A first principles computational study, Doctorate, T.İRİFAN(Student), 2017

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

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

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

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

AKATA KURÇ B., TOFFOLÌ H., Modelling and experimental study of titanosilicate ETS-10: application for solar cells, Post Graduate, M.KOÇ(Student), 2013

TOFFOLÌ H., Investigation of catalytic properties and electronic structure of correlated material CeO₂ with ab-initio computational methods, Post Graduate, B.ÖZDEMİR(Student), 2013

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

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

TOFFOLÌ H., Density functional theory investigation of noble metal reduction agents on γ -aluminum oxide in NOx storage/reduction catalysts, Post Graduate, Z.ARTUÇ(Student), 2011

TOFFOLÌ H., The effects of promoters on the sulfur resistance of NOx storage/reduction catalysts: A density functional theory investigation, Post Graduate, R.KOŞAK(Student), 2011

TOFFOLÌ H., Effect of support material in NOx storage/reduction catalysts, Post Graduate, R.HUMMATOV(Student), 2010

TOFFOLÌ H., Density functional theory investigation of TiO₂ anatase nanosheets, Post Graduate, C.SİBEL(Student), 2009

TOFFOLÌ H., Density functional theory for trapped ultracold fermions, Post Graduate, Ö.AKYAR(Student), 2009

TOFFOLÌ H., Electronic properties of dye molecules adsorbed on anatase-titania surface for solar cell applications, Post Graduate, E.TORUN(Student), 2009

Articles Published in Journals That Entered SCI, SSCI and AHCI Indexes

- **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 (Journal Indexed in SCI)
- **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, pp.28411-28418, 2019 (Journal Indexed in SCI)
- **Combined effect of point defects and layer number on the adsorption of benzene and toluene on graphene**
Akay T. I. , Toffoli D., TOFFOLÌ H.
APPLIED SURFACE SCIENCE, vol.480, pp.1063-1069, 2019 (Journal Indexed in SCI)
- **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, pp.19678-19686, 2018 (Journal Indexed in SCI)
- **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, pp.7976-7984, 2017 (Journal Indexed in SCI)
- **Electronic properties of the boroxine-gold interface: evidence of ultra-fast charge delocalization**
Toffoli D., Stredansky M., Feng Z., Balducci G., Furlan S., Stener M., Ustunel H., Cvetko D., Kladnik G., Morgante A., et al.
CHEMICAL SCIENCE, vol.8, pp.3789-3798, 2017 (Journal Indexed in SCI)
- **Structural and electronic properties of bulk and low-index surfaces of zincblende PtC**
Sensoy M. G. , Toffoli D., TOFFOLÌ H.
JOURNAL OF PHYSICS-CONDENSED MATTER, vol.29, 2017 (Journal Indexed in SCI)
- **Comparative Analysis of Reactant and Product Adsorption Energies in the Selective Oxidative Coupling of Alcohols to Esters on Au(111)**
Senozan S., TOFFOLÌ H., Karatok M., Vovk E. I. , Shah A. A. , ÖZENSOY E., Toffoli D.
TOPICS IN CATALYSIS, vol.59, pp.1383-1393, 2016 (Journal Indexed in SCI)
- **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 (Journal Indexed in SCI)
- **Active role of the support in NOx storage and reduction catalytic systems**
Tek M., TOFFOLÌ H., Toffoli D.

- APPLIED SURFACE SCIENCE, vol.355, pp.1295-1305, 2015 (Journal Indexed in SCI)
Covalent and noncovalent functionalization of pristine and defective graphene by cyclohexane and dehydrogenated derivatives
 Sayin C. S., Toffoli D., TOFFOLÌ H.
- APPLIED SURFACE SCIENCE, vol.351, pp.344-352, 2015 (Journal Indexed in SCI)
Understanding the Effects of Ion-Exchange in Titanosilicate ETS-10: A Joint Theoretical and Experimental Study
 Koc M., Galioglu S., Toffoli D., TOFFOLÌ H., AKATA KURÇ B.
- JOURNAL OF PHYSICAL CHEMISTRY C, vol.118, pp.27281-27291, 2014 (Journal Indexed in SCI)
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, pp.22522-22532, 2014 (Journal Indexed in SCI)
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 (Journal Indexed in SCI)
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, pp.48492-48506, 2014 (Journal Indexed in SCI)
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., TOFFOLÌ H.
- JOURNAL OF PHYSICAL CHEMISTRY C, vol.116, pp.6191-6199, 2012 (Journal Indexed in SCI)
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, 2010 (Journal Indexed in SCI)
The self-consistent calculation of exchange enhanced odd integer quantized Hall plateaus within Thomas-Fermi-Dirac approximation
 Bilgec G., TOFFOLÌ H., Siddiki A., SÖKMEN İ.
- PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES, vol.42, pp.1058-1061, 2010 (Journal Indexed in SCI)
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, pp.926-932, 2009 (Journal Indexed in SCI)
High-capacity hydrogen storage by metallized graphene
 Ataca C., Akturk E., ÇIRACI S., Ustunel H.
- APPLIED PHYSICS LETTERS, vol.93, 2008 (Journal Indexed in SCI)
Structural properties and stability of nanoclusters
 Ustunel H., Erkoc S.
- JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, vol.4, pp.928-956, 2007 (Journal Indexed in SCI)
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, 2007 (Journal Indexed in SCI)
Modeling a suspended nanotube oscillator
 Ustunel H., Roundy D., Arias T.
- NANO LETTERS, vol.5, pp.523-526, 2005 (Journal Indexed in SCI)

- **Ab initio mechanical response: Internal friction and structure of divacancies in silicon**
Ustunel H., Roundy D., Arias T.
PHYSICAL REVIEW LETTERS, vol.94, 2005 (Journal Indexed in SCI)
- **A tunable carbon nanotube electromechanical oscillator**
Sazonova V., Yaish Y., Ustunel H., Roundy D., Arias T., McEuen P.
NATURE, vol.431, pp.284-287, 2004 (Journal Indexed in SCI)
- **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, pp.517-520, 2004 (Journal Indexed in SCI)

Refereed Congress / Symposium Publications in Proceedings

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

Supported Projects

- TOFFOLÍ H., NATO Supported Research Project, Advanced Microwave Sources, 2017 - 2018
- TOFFOLÍ H., DEMİRTAŞ M., Project Supported by Higher Education Institutions, SU-GAZ DEĞİŞİMİ MEKANİZMASININ YÜK YOĞUNLUĞU FONKSİYONELİ TEORİSİYLE İNCELENMESİ, 2013 - 2013
- TOFFOLÍ H., ŞENSOY M. G. , Project Supported by Higher Education Institutions, SU-GAZ DEĞİŞİMİ REAKSİYONUNDA ALTTAŞ MALZEMENİN ETKİSİNİN YÜK YOĞUNLUĞU FONKSİYONELİ KULLANILARAK İNCELENMESİ, 2013 - 2013
- TOFFOLÍ H., Project Supported by Higher Education Institutions, Yariletken Nanotellerin Manyetik Atomlarla Katkılandırılması Konusunda Yük Yoğunluğu Fonksiyoneli Hesapları, 2009 - 2009

Citations

Total Citations (WOS):2163
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