

Hande Toffoli

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Curriculum Vitae

General

Born May 6th, 1977 in Ankara (Turkey)
Citizenship Turkish
Web page <http://physics.metu.edu.tr/~hande>

Education

1999-2005 **PhD in Physics**, *Cornell University*, Ithaca, NY, USA.
1995-1999 **BSc in Physics (3.91/4.00, ranked first in the department)**, *Middle East Technical University*, Ankara, Turkey.

Employment

2013-present Associate Professor (awarded by the Turkish Board of Higher Education)
2007-2013 Assistant Professor, Department of Physics, Middle East Technical University
2006-2007 Instructor, Department of Physics, Middle East Technical University
2005-2006 Postdoctoral Fellow, ISAS/SISSA (International School of Advanced Studies), Italy
2000-2005 Research Assistant, Department of Physics, Cornell University, USA
1999-2000 Teaching Assistant, Department of Physics, Cornell University, USA

Languages

Turkish **Native speaker**
English **Advanced TOEFL: 117/120**
Italian **Intermediate**

Teaching

Physics 101 Physics for Non-Scientists I
Physics 102 Physics for Non-Scientists II
Physics 105 General Physics I
Physics 106 General Physics II
Physics 113 Introductory Physics for physics students I (mechanics)
Physics 114 Introductory Physics for physics students II (electricity and magnetism)
Physics 181 Basic Physics I
Physics 112 Physics II
Physics 200 Basics of scientific computing, **co-designed with colleague**
Physics 343 Introduction to Computational Techniques for Physicists, **own design**
Physics 429 Statistical Mechanics, **honors' roll**
Physics 430 Statistical Thermodynamics
Physics 501 Statistical Mechanics, **graduate level**
Physics 531 Solid State I, **graduate level**

Physics 533 Many-Body Physics I, **graduate level**

Physics 741 Principles of Density Functional Theory **own design, graduate level**

Computer Skills

Octave/Matlab, Python, Shell scripting

C, Fortran

Linux, Latex

Publications (refereed journals)

1. "The Effect of Platinum, Gold and Potassium Additives on the Surface Chemistry of CdI₂ Antitype Mo₂C", M. Demirtas, H. Ustunel, D. Toffoli *ACS Omega*, accepted for publication (2017)
2. "Electronic Properties of the Boroxine-Gold Interface: Evidence of Ultra-Fast Charge Delocalization", D. Toffoli *et al. Chem Sci*, **8**, (2017) 3789–3789
3. "Structural and Electronic Properties of Bulk and Low-Index Surfaces of Zincblende PtC", M. G. Sensoy, D. Toffoli, H. Ustunel, *J Phys: Cond Matt* **29** (2017) 125002
4. "Comparative Analysis of Reactant and Product Adsorption Energies in the Selective Oxidative Coupling of Alcohols to Esters on Au(111)", S. Senozan, H. Ustunel, M. Karatok, E. I. Vovk, A. A. Shah, E. Ozensoy, D. Toffoli, *Top Catal*, **59** (2016) 1383–1393
5. "Multiscale Self-Assembly of Silicon Quantum Dots into an Anisotropic Three-Dimensional Random Network", S. Ilday, F. O. Ilday, R. Hubner, T. J. Prosa, I. Martin, G. Nogay, I. Kabacelik, Z. Mics, M. Bonn, D. Turchinovich, H. Toffoli, D. Toffoli, D. Friedrich, B. Schmidt, K.-H. Heinig, and R. Turan *Nano Letters*, **16**, (2016) 1942–1948
6. "Active role of the support in NO_x storage and reduction catalytic systems", M. Tek, H. Ustunel, D. Toffoli *Applied Surface Science*, **355** (2015) 1295-1305
7. "Covalent and Noncovalent Functionalization of Pristine and Defective Graphene by Cyclohexane and Dehydrogenated Derivatives", C. S. Sayin, D. Toffoli, H. Ustunel, *Applied Surface Science*, **351** (2015) 344-352
8. "Understanding the Effects of Ion-Exchange in Titanosilicate ETS-10: A Joint Theoretical and Experimental Study", M. Koc, S. Galioglu, D. Toffoli, H. Ustunel, B. Akata *Journal of Physical Chemistry C*, **118** (2014), 27281-27291
9. "First principles investigation of NO₂ and SO₂ adsorption on γ -Al₂O₃ supported mono- and diatomic metal clusters", Z. Artuc, H. Ustunel, D. Toffoli *RSC Advances* **4**, 48492-48506 (2014)
10. "Bis(triisopropylsilylethynyl)pentacene/Au(111) Interface: Coupling, Molecular Orientation, and Thermal Stability", A. Gnoli, H. Ustunel, D. Toffoli, L. Yu, D. Catone, S. Turchini, S. Lizzit, N. Stingelin, R. Larciprete *Journal of Physical Chemistry C* **118**, 22522-22532 (2014)
11. "Insights into surface-adsorbate interactions in corrosion inhibition processes at the molecular level", M. Ozcan, D. Toffoli, H. Ustunel, I. Dehri *Corrosion Science* **80**, 482-489 (2014)
12. "First-Principles Investigation of NO_x and SO_x Adsorption on Anatase-Supported BaO and Pt

Overlayers", R. Hummatov , O. Gulseren; E. Ozensoy ; D. Toffoli, H. Üstünel, *Journal of Physical Chemistry C*, **116** 6191-6199 (2012)

13. "Metallization of C₆₀/Rh(100) interface revealed by valence photoelectron spectroscopy and density functional theory calculations", A.-C. Wade, S. Lizzit, L. Petaccia, A. Goldoni, D. Diop, H. Üstünel, S. Fabris, S. Baroni, *Journal of Chemical Physics*, **132** 234710 (2010)
14. "The self-consistent calculation of exchange enhanced odd integer quantized Hall plateaus within Thomas-Fermi-Dirac approximation", G. Bilgec, H. Üstünel Toffoli, A. Siddiki, I. Sokmen, *Physica E*, **42** 1058-1061 (2010)
15. "Structural, electronic and magnetic properties of BN nanotubes doped with Mn and Cr : exploring the potential for device technology" by H. Kökten, H. Üstünel and Ş. Erkoç, *Journal of Computational and Theoretical Nanoscience*, **6**, 926-932 (2009)
16. "High-capacity hydrogen storage by metallized graphene", Ataca C, Akturk E, Ciraci S, H. Üstünel *Applied Physics Letters* **93** 043123 (2008)
17. "Defect-controlled transport properties of metallic atoms along carbon nanotube surfaces," by A. Barinov, H. Üstünel, S. Fabris, L. Gregoratti, L. Aballe, P. Dudin, S. Baroni, M. Kiskinova *Physical Review Letters* **99**, 046803-(1-4) (2007).
18. "Structural Properties and Stability of Nanoclusters," by H.Üstünel and Ş. Erkoç *Journal of Computational and Theoretical Nanoscience* **4** 1-29 (2007)
19. "Modelling a suspended nanotube oscillator," by H.Üstünel, D. Roundy and T. A. Arias *Nano Letters* **5** 523–526 (2005)
20. "*Ab initio* mechanical response: internal friction and structure of divacancies in silicon," by H. Üstünel, D. Roundy and T.A. Arias, *Physical Review Letters*, **94**, 025503 (2005).
21. "A tunable carbon nanotube electromechanical oscillator," by V. Sazonova, Y. Yaish, H. Üstünel, D. Roundy, T.A. Arias and P.L. McEuen, *Nature*, **431**, 284–287 (2004).
22. "Electron-phonon scattering in metallic single-walled carbon nanotubes", by J.-Y. Park, S. Rosenblatt, Y. Yaish, V. Sazonova, H. Üstünel, S. Braig, T.A. Arias, P. Brouwer and P. L. McEuen, *Nano Lett.* **4**, 517–520 (2004).

Citation metrics compiled via ISI Web of Science (as of October, 2017)

- Citations (excluding self citations): >1700
- h-index: 7

Publications (book chapter)

- H. Toffoli, S. Erkoç, D. Toffoli, J. Leszczynski, *Handbook of Computational Chemistry (Modeling of Nanostructures)*, pp. 995-1041, Germany, Springer Science+Business Media B.V, 2012.

Publications (conference proceedings, brief refereed papers)

- "Density Functional Theory Approach to Trapped Dipolar Fermions", *IOP Journal of Physics: Conference Series*, **in press** (2014), B. Tanatar, [H. Ustunel](#), S. Abedinpour
- "Effect of ion-exchange on Structural, Electronic, and Vibrational Properties of the -O-Ti-O-Ti-O-Quantum Wires in ETS-10", *MRS Proceedings*, **1704** (2014), M. Koc, D. Toffoli, [H. Ustunel](#), B. Akata

Awards

- 2010 METU Young Researcher Performance Award
- 2012 METU Young Researcher Performance Award
- 2015 METU Young Researcher Performance Award
- 2015 BAGEP (Turkish Academy of Sciences) Young Researcher Award

Mentoring activity

Post-doctoral researcher

- Selma Bas (Completed)

PhD students – Single advisor

- Ceren Sibel Sayın (Physics, completed)

PhD students – Main advisor

- Mehmet Gokhan Sensoy (Physics, completed)
- Merve Demirtas (Physics, ongoing)
- Mustafa Tek (Physics, transferred)

PhD students — Co-advisor

- Tugce Irfan Ersoz (MNT, completed)
- Seda Kibar (MNT, terminated)

MSc students — Single advisor

- Gozdenur Toraman (Physics, ongoing)
- Firat Yalcin (Physics, ongoing)
- Gizem Senturk (Physics, ongoing)
- Ozge Akyar (Physics, completed)
- Burak Ozdemir (Physics, completed)
- Okan Karaca Orhan (Physics, completed)

MSc students — Main advisor

- Ceren Sibel Sayın (Physics, completed)
- Ruslan Hummatov (Physics, completed)
- Gokce Sokmen (MNT, completed)
- Engin Torun (Physics, completed)
- Ozan Dernek (Physics, ongoing)

MSc students — Co-advisor

- Zuleyha Artuc (MNT, completed)
- Mehmet Koc (MNT, completed)
- Rukan Kosak (Chemistry, completed)

Selected Oral and Poster Presentations — presenting

- APS March Meeting, Indianapolis, USA March, **2002**, *Ab initio mechanical response: determination of the structure of the silicon divacancy*
- Electronic Structure Conference, San Francisco, USA June, **2002**, poster presentation
- APS March Meeting, Montreal, Canada March, **2004**, *Electron-optic phonon interactions in carbon nanotubes*
- APS March Meeting, Los Angeles, USA March, **2005**, *Theory of vibrations in suspended nanotubes*
- NanoItaly, Trieste, Italy May, **2006**, *Indium migration through a nanotube forest: fingerprinting the diffusing species by combining DFT and XPS data*
- Nano-TR, Ankara, Turkey, **2007**, *Density-Functional Modeling of X-ray Photoemission Spectroscopy: an Application to the Diffusion of Indium on Multi-Walled Carbon Nanotubes (invited)*
- Istanbul Statistical Physics Days, Istanbul, Turkey, **2007**, *Density Functional Modeling of Photoemission (invited)*
- ECOS-29, Edinburgh, Scotland, **2012**, *Designing storage and reduction catalysts with improved sulfur tolerance: an ab-initio study on γ -Al₂O₃ supported bimetallic systems*
- Chemistry Via Computation (invited talk), Istanbul, Bogazici University,

Selected Oral and Poster Presentations — not presenting

- APS, March Meeting, Denver, Colorado, USA March, **2014**, *Density functional theory investigation of cyclohexane as a potential functionalizing agent on graphene*, C. S. Sayin, D. Toffoli, H. Ustunel
- APS, March Meeting, Denver, Colorado, USA March, **2014**, *Density Functional Theory Investigation of Adsorption Properties of CO, CO₂ and H₂O on γ -Al₂O₃ Supported Pt Clusters*, M. Tek, H. Ustunel, D. Toffoli
- APS, March Meeting, Denver, Colorado, USA March, **2014**, *Density Functional Theory Investigation of Adsorption Properties of CO, CO₂ and H₂O on γ -Al₂O₃ Supported Pt Clusters*, M. G. Sensoy, H. Ustunel, D. Toffoli
- MRS Spring Meeting, San Francisco, California, USA April, **2014**, *Effect of ion-exchange on Structural, Electronic, and Vibrational Properties of the -O-Ti-O-Ti-O- Quantum Wires in ETS-10*, M. Koc, D. Toffoli, H. Ustunel, B. Akata
- 27th Conference on Low Temperature Physics, Buenos Aires, Argentina, August, **2014**, *Density Functional Theory Approach to Trapped Dipolar Fermions*, B. Tanatar, H. Ustunel, S. Abedinpour
- Nano2016, Quebec City, Canada, **2016**, *Density functional theory investigation of the Ni- and Rh-doped Au(111) surface as a viable catalyst for selective oxidation of ethanol*, O. Dernek, D. Toffoli, H. Ustunel

Project Work

- TÜBİTAK 1001 Project No: 108T706 entitled 'Yoğunluk fonksiyoneli teorisine dayanan temel prensip hesabı ile Pt/BaO/Al₂O₃ NOX indirgeme/depolama katalizörünün işleme mekanizmasının incelenmesi ve verimliliştirilmesi' as Principal Investigator (completed)
- TÜBİTAK 1001 Project No: 107T142 entitled 'Çok parçacıklı sistemlerin geometri optimizasyonu için paralel kod geliştirilmesi: Nano-sistemlerde hidrojen depolama ve nano ölçekli mıknatıs yapılarının incelenmesi uygulamaları' as Researcher (completed)
- TÜBİTAK 1001 Project No: 109T105 entitled 'Metal Nanotellerin Mekanik, Termodinamik ve Elektronik Özellikler' as Advisor (completed)
- TÜBİTAK 1001 Project No: 112T542 'Yakıt Gözesi Uygulamaları için H₂ Üretimde Kullanılan Yüksek Aktiviteli Katalizörlerin Yük Yoğunluğu Fonksiyoneli Teorisi Kullanılarak Tasarlanması' as

Researcher (completed)

- TÜBİTAK-CNR Bilateral project No : 113F377 entitled 'Fotoiyonizasyonda Çok-Elektronlu Süreçlerin Teorik Olarak İncelenmesi' as Researcher (ongoing)
- TÜBİTAK 1001 Project No: 113F099 entitled 'Altın Katalizörler Üzerinde Alkollerin Seçici Oksitlenmesi Reaksiyon Mekanizmalarının Yük Yoğunluğu Fonksiyoneli Teorisi Ile İncelenmesi' as Principal Investigator (ongoing)
- TÜBİTAK 1001 Project No: 115F493 entitled 'A joint theoretical and experimental study on the nanotribological properties of the interface between Au and two-dimensional systems' as Principal Investigator (ongoing)

Workshop organizer

- IARS Frontiers Workshop on DFT and its applications in Nanosciences, Turunc-Marmaris, 19-29 October 2009
- International Winter School of Applications of Computer Simulation and Modelling in Contemporary Solid State Physics and Nanotechnology, Institute of Theoretical and Applied Physics (ITAP), Turunc, Marmaris 28 January - 6 February 2008

Peer review activity

- Three NSF grants
- TÜBİTAK 1001/1305 project panels, external consultant
- Several journal papers
 - Journal of Physical Chemistry (1 paper, 2015)
 - Applied Surface Science (1 paper, 2015)
 - Frontiers in Physics (1 review paper, 2016)
 - Materials Research Express (1 paper, 2016)
 - Journal of Applied Physics (1 paper, 2017)

Book review

- Technical review of a computer-language book for CRC Publishing, 2014

Other responsibilities

2017-present Vice department chair

2016-present PhD Qualifier Exam Preparation Committee — responsible for the Statistical Mechanics exam.

2012-2015 Advisor to the department chair

2008-present Faculty member in the Program of Micro and Nanotechnology