

# CURRICULUM VITAE

(March 2013)

## Şinasi S. Ellialtıođlu

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### PERSONAL DATA :

Date of Birth : November 4, 1950  
Place of Birth : Ankara, Turkey

### EDUCATION :

- B.S. 1971 Middle East Technical University, Ankara
- M.S. 1973 Middle East Technical University, Ankara
- Ph.D. 1977 University of Missouri, Columbia, MO
- Dozentship 1982 Middle East Technical University, Ankara

### HONORS :

- Fellowship of Turkish Ministry of Education  
(Haydarpaşa Lisesi, İstanbul 1961–1964)  
(Science Lycée, Ankara 1964–1967)
- J. F. Kennedy Fellowship for Basic Sciences (1967–1971)  
Middle East Technical University, Ankara
- O. M. Stewart Fellowship (1975, 1976, 1977)  
University of Missouri–Columbia, MO
- Research Fellowship of Rockwell Int. Corp. (1976)  
University of Missouri–Columbia, MO
- Scholarship – Graduate School Dean (1977)  
University of Missouri–Columbia, MO
- Postdoctoral Fellow of National Science Foundation (1978–1979, 1980)  
University of Missouri–Columbia, MO
- Research Fellow of Alexander von Humboldt Stiftung (1984–1985, 1986)  
Institut für Festkörperforschung der Kernforschungsanlage (IFF–KFA), Jülich

- TÜBİTAK–Incentive Award in Science (1987)  
Scientific and Technical Research Council of Turkey
- NATO–B Scientific Research Fellow (1995)  
Georgia Institute of Technology, Atlanta, GA
- Fulbright Research Fellow (1995–1996)  
Georgia Institute of Technology, Atlanta, GA

#### **WORK EXPERIENCE :**

- Assistant : 1971–1973 METU–Physics Department, Ankara  
1973–1974 Southern Illinois University–Carbondale, IL  
1974–1977 University of Missouri–Columbia, MO
- Instructor, Dr. : 1978–1980 METU–Physics Department, Ankara
- Assist. Prof. Dr. : 1980–1982 METU–Physics Department, Ankara
- Assoc. Prof. Dr. : 1982–1988 METU–Physics Department, Ankara
- Professor Dr. : 1988–2012 METU–Physics Department, Ankara
- Professor Dr. : 2012– TEDU–Basic Sciences Unit, Ankara

#### **ADMINISTRATIVE EXPERIENCE :**

- National Administrator of Turkey (1988–1989)  
NATO Science Fellowship Programme
- Member and the Chairman (1988–1989)  
Executive Committee of the Group for Raising Scientists  
Scientific and Technical Research Council of Turkey (TÜBİTAK)
- Chairman of the Physics Department (1988–1994)  
Middle East Technical University
- Member of the University Administration Board (1992–1994)  
Middle East Technical University
- Member of the University Academic Publishing Committee (1993–1994)  
Middle East Technical University
- Member of the Advisory Board  
to the Turkish Atomic Energy Authority (1993–1996)
- Member of the Advisory Board  
to the European High Pressure Research Group (1993–1996)
- Member of the Publication Evaluation Commission  
of the Turkish Universities (1993–2009)
- Member of the Advisory Committee  
to the Feza Gürsey Science Center (1993–1994)
- Director of Basic Sciences Unit  
TED University (2012– )

## **OTHER ACTIVITIES :**

- Consultant to Amoco Research Center, Naperville, IL (1985)
- International Physics Olympiad (1986, 1987)  
Selection and Training of the Turkish National Team
- Organizer of the Spring School on “Surface Science and Technology”  
1988, Bilkent University, Ankara
- Organizer of the International Conference on “Beam–Solid Interactions”  
1989, METU, Ankara
- Organizer of the 2nd National Symposium on “Computer Simulations”  
1990, METU, Ankara
- Organizer of the Ankara Conferences on “Condensed Matter Physics” (YMF)  
YMF02 1992, Bilkent University, Ankara  
YMF03 1993, Ankara University, Ankara  
YMF05 1997, METU, Ankara (Principal Organizer)  
YMF06 1997, Gazi University, Ankara  
YMF07 1998, Bilkent University, Ankara  
YMF08 2001, Bilkent University, Ankara  
YMF09 2002, Bilkent University, Ankara  
YMF10 2003, Hacettepe University, Ankara  
YMF11 2004, Gazi University, Ankara  
YMF12 2005, Ankara University, Ankara  
YMF13 2006, METU, Ankara (Principal Organizer)  
YMF14 2007, Hacettepe Üniversitesi, Ankara  
YMF15 2008, Bilkent Üniversitesi, Ankara  
YMF16 2009, Gazi Üniversitesi, Ankara  
YMF17 2010, Ankara Üniversitesi, Ankara  
YMF18 2011, METU, Ankara (Principal Organizer)
- Organizer of the 1st Anatolian School on “Catalysis”  
2006, METU, Ankara

## **PROFESSIONAL AFFILIATIONS :**

- Member of the Turkish Physical Society
- Member of the Materials Research Society
- Member of the Humboldtians’ Association of Turkey
- Member of the Fulbright Fellows Association of Turkey
- Member of the METU Alumni Association
- Member of the Ankara Science Lycée Alumni Association

# LIST OF PUBLICATIONS

## BOOK :

- “Electronic and Optical Properties of d-Band Perovskites”  
T. Wolfram and Ş. Ellialtıođlu  
(Cambridge University Press, Cambridge, 2006). pp.1–315. [7 in 2012]
- “Applications of Group Theory to Atoms, Molecules, and Solids”  
T. Wolfram and Ş. Ellialtıođlu  
(Cambridge University Press, Cambridge), 533+ pages,  
accepted, in process of typesetting and production,  
expected physical stock date: October 2013.

## EDITED VOLUME :

- “Proceedings of the International Conference on Beam–Solid Interactions”  
R. Ellialtıođlu and Ş. Ellialtıođlu (Guest Editors)  
Turkish J. of Phys., Supplement No.1, pp. 1–246, February 1990, Ankara

## EDITED CHAPTER :

- “Concepts of Surface States and Chemisorption on d-Band Perovskites”  
T. Wolfram and Ş. Ellialtıođlu  
Chapter 6 in “Theory of Chemisorption”, ed. J. R. Smith  
Volume **19** of Topics in Current Physics, (Springer–Verlag, Heidelberg, 1980)  
pp. 149–181. [24]

## ARTICLES in SCI :

1. “Surface Enhanced Covalency and its Effects on the Surface States  
of d-Band Metal Oxides”  
T. Wolfram and Ş. Ellialtıođlu  
Appl. Phys. **13**, 21 (1977). [**Number of citations** = 30]
2. “Electronic Density of States for the Perovskites”  
Ş. Ellialtıođlu and T. Wolfram  
Phys. Rev. B **15**, 5909 (1977). [25]
3. “Surface Electronic Properties of d–Band Perovskites: Study of  $\pi$ -Bands”  
Ş. Ellialtıođlu and T. Wolfram  
Phys. Rev. B **18**, 4509 (1978). [34]
4. “Surface States on n-type SrTiO<sub>3</sub>”  
Ş. Ellialtıođlu, T. Wolfram, and Victor E. Henrich  
Solid State Commun. **27**, 321 (1978). [21]
5. “Model for the x-ray Photoelectron Distributions of d-Band Perovskites”  
T. Wolfram and Ş. Ellialtıođlu  
Phys. Rev. B **19**, 43 (1979). [18]
6. “Matrix Element Effects in  $\epsilon_2(\omega)$  of the Insulating Perovskites”  
T. Wolfram and Ş. Ellialtıođlu  
Appl. Phys. **22**, 11 (1980). [1]

7. “Neutron Scattering by Magnons of an Antiferromagnet with Modulated Spin Amplitudes”  
T. Wolfram and Ş. Ellialtıođlu  
Phys. Rev. Lett. **44**, 1295 (1980). [13]
8. “Electronic Structure of SiO<sub>2</sub>(111) Thin Film”  
S. ıracı and Ş. Ellialtıođlu  
Solid State Commun. **40**, 587 (1981). [12]
9. “An Investigation of the Interface Electronic Structure of Si–SiO<sub>2</sub> Junctions”  
S. ıracı, Ş. Ellialtıođlu, and Ş. Erko  
J. Vac. Sci. Technol. **21**, 402 (1982). [4]
10. “Density-of-States and Partial-Density-of-States Functions for the Cubic d-Band Perovskites”  
T. Wolfram and Ş. Ellialtıođlu  
Phys. Rev. B **25**, 2697 (1982). [33]
11. “Surface Electronic Structure of Silicon Dioxide”  
S. ıracı and Ş. Ellialtıođlu  
Phys. Rev. B **25**, 4019 (1982). [20]
12. “Interpretation of the Spectra Obtained from Oxygen Adsorbed and Oxidized Silicon Surfaces”  
S. ıracı, Ş. Ellialtıođlu, and Ş. Erko  
Phys. Rev. B **26**, 5716 (1982). [70]
13. “Chemisorption of Atomic Oxygen on Silicon Surfaces”  
Ş. Ellialtıođlu and S. ıracı  
Solid State Commun. **42**, 879 (1982). [7]
14. “States of Water Molecule Adsorbed on Si(111) Surface”  
S. ıracı, Ş. Erko, and Ş. Ellialtıođlu  
Solid State Commun. **45**, 35 (1983).
15. “Binding Energy of Donor–Phonon System in Quantum Well Wires”  
A. Erelebi, U. zdiner and Ş. Ellialtıođlu  
J. Phys. C **19**, L67 (1986). [5]
16. “Magnetic 3d-impurities in Nb and Mo”  
Ş. Ellialtıođlu, R. Zeller, and P. H. Dederichs  
J. Phys. F **17**, 409 (1987). [12]
17. “Electronic Structure of Strained Si<sub>n</sub>/Ge<sub>n</sub>(001) Superlattices”  
S. ıracı, O. Glseren, and Ş. Ellialtıođlu  
Solid State Commun. **65**, 1285 (1988). [3]
18. “Calculations of STM Linescans – General Formalism”  
Ş. Ellialtıođlu, S. ıracı, and Inder P. Batra  
Solid State Commun. **66**, 1135 (1988). [4]
19. “A Computer Simulation of Amorphous Silicon”  
G. Dereli, M. C. Yalabık, and Ş. Ellialtıođlu  
Physica Scripta **40**, 117 (1989). [2]

20. “Elastic Properties of  $\text{GaS}_{1-x}\text{Se}_x$  Layer Mixed Crystals by Brillouin Scattering”  
N. M. Gasanly, B. G. Akınođlu, and Ő. Ellialtıođlu  
*Phys. Stat. Sol. (b)* **177**, K59 (1993). [1]
21. “Raman Scattering in Layer Indium Selenide under Pressure”  
K. Allahverdi, S. Babaev, Ő. Ellialtıođlu, and A. Ismailov  
*Solid State Commun.* **87**, 675 (1993). [6]
22. “Low-Temperature Phase Transitions in  $\text{TlGaS}_2$  Layer Crystals”  
A. Aydınlı, R. Ellialtıođlu, K. R. Allakhverdiev, Ő. Ellialtıođlu, and N. M. Gasanly  
*Solid State Commun.* **88**, 387 (1993). [13]
23. “Elastic Coefficients in  $\text{TlGa}(\text{S}_{1-x}\text{Se}_x)_2$  and  $\text{TlIn}_x\text{Ga}_{1-x}\text{S}_2$  Layer Mixed Crystals  
by Brillouin Scattering”  
N. M. Gasanly, B. G. Akınođlu, Ő. Ellialtıođlu, R. Laiho, and A. E. Bakhyshev  
*Physica B* **192**, 371 (1993). [8]
24. “Lattice Parameters of  $\text{TlGa}_{1-x}\text{In}_x\text{S}_2$  and  $\text{TlGa}(\text{S}_{1-x}\text{Se}_x)_2$  Layer Mixed Crystals”  
N. M. Gasanly, A. Çulfaz, H. Özkan, and Ő. Ellialtıođlu  
*Cryst. Res. Technol.* **29**, K51 (1994). [5]
25. “Chemisorption of a p-adsorbate on perovskites”  
H. Kökten and Ő. Ellialtıođlu  
*Physica B* **193**, 39 (1994).
26. “Low-Temperature Second Harmonic Generation in Gallium Selenide  
under Resonant Excitation of the Direct Free Excitons”  
K. Allakhverdiev, N. Akhmedov, Z. Ibragimov, Ő. Ellialtıođlu,  
K. Lothar, and D. Haarer  
*Solid State Commun.* **93**, 147 (1995). [5]
27. “Layered Semiconductor GeS as Birefringent Stratified Medium”  
R. A. Süleymanov, Ő. Ellialtıođlu, and B. G. Akınođlu  
*Phys. Rev. B* **52**, 7806 (1995). [3]
28. “Spatial Stabilization of Townsend and Glow Discharges with a Semiconducting  
Cathode”  
B. G. Salamov, Ő. Ellialtıođlu, B. G. Akınođlu, N. N. Lebedeva, and L. G. Patriskii  
*J. Phys. D: Appl. Phys.* **29**, 628 (1996). [32]
29. “Ab initio Study of Adsorption and Desorption of Se on the Si(001) Surface”  
M. Çakmak, G. P. Srivastava, Ő. Ellialtıođlu, and K. Çolakođlu  
*Surf. Sci.* **507–510**, 29 (2002). [3]
30. “Adsorption of Te on Ge(001) : Density-functional calculations”  
M. Çakmak, G. P. Srivastava, and Ő. Ellialtıođlu  
*Phys. Rev. B* **67**, 205314 (2003). [5]
31. “Ab initio study of the one-monolayer Sb/Si(001) interface”  
M. Çakmak, R. Shaltaf, G. P. Srivastava, and Ő. Ellialtıođlu  
*Surf. Sci.* **532–535**, 661 (2003). [4]
32. “Electronic and structural properties of a 4d perovskite: Cubic phase of  $\text{SrZrO}_3$ ”  
E. Mete, R. Shaltaf, and Ő. Ellialtıođlu  
*Phys. Rev. B* **68**, 035119 (2003). [44]

33. “Mg adsorption on Si(001) surface from first principles”  
R. Shaltaf, E. Mete, and Ş. Ellialtıođlu  
Phys. Rev. B **69**, 125417 (2004). [7]
34. “An ab initio study of the Te surfactant on Ge/Si(001)”  
M. akmak, G. P. Srivastava, and Ş. Ellialtıođlu  
Surf. Sci. **566–568**, 719 (2004).
35. “Ab initio study of the one-monolayer Sb/Ge(001) interface”  
R. Shaltaf, M. akmak, E. Mete, G. P. Srivastava, and Ş. Ellialtıođlu  
Surf. Sci. **566–568**, 956 (2004).
36. “Electronic structure of the chainlike compound TlSe”  
Ş. Ellialtıođlu, E. Mete, R. Shaltaf, K. Allakhverdiev, F. Gashimzade,  
M. Nizamettinova, and G. Orudzhev  
Phys. Rev. B **70**, 195118 (2004). [14]
37. “DFT study of Rb/Si(100)-2×1 System”  
E. Mete, R. Shaltaf and Ş. Ellialtıođlu  
Surf. Sci. **583**, 119 (2005). [2]
38. “Cs adsorption on Si(001) surface : ab initio study”  
R. Shaltaf, E. Mete and Ş. Ellialtıođlu  
Phys. Rev. B **72**, 205415 (2005). [6]
39. “Lattice vibrations of pure and doped GaSe”  
K. Allakhverdiev, T. Baykara, Ş. Ellialtıođlu, F. Hashimzade,  
D. Huseinova, K. Kawamura, A. A. Kaya, A. M. Kulibekov, and S. Onari  
Mater. Res. Bull. **41**, 751 (2006). [8]
40. “Atomic and electronic structures of Sr/Si(001)-2×2”  
M. akmak, E. Mete, and Ş. Ellialtıođlu  
Surf. Sci. **600**, 3614 (2006). [2]
41. “Effect of hydrogenation on B/Si(001)-1×2”  
M. Cakmak, E. Mete, and Ş. Ellialtıođlu  
Surf. Sci. **601**, 3711 (2007).
42. “An ab initio study of 3-aminopropyltrimethoxysilane molecule  
on Si(111)-( $\sqrt{3} \times \sqrt{3}$ ) surface”  
G. Demirel, G. Birlik, M. Cakmak, T. Caykara, and Ş. Ellialtıođlu  
Surf. Sci. **601**, 3740 (2007). [5]
43. “Effect of molecular and electronic structure on the light-harvesting properties  
of dye sensitizers”  
E. Mete, D. Uner, M. Cakmak, O. Gulseren, Ş. Ellialtıođlu  
J. Phys. Chem. C **111**, 7539 (2007).
44. “Chemisorption of 3-aminopropyltrimetoxysilane on Si(001)-(2×2)”  
G. Demirel, M. akmak, T. aykara, Ş. Ellialtıođlu  
J. Phys. Chem. C **111**, 15020 (2007). [6]
45. “Atomic and electronic structure of Bi/GaAs(001)- $\alpha 2(2 \times 4)$ ”  
D. Usanmaz, M. Cakmak, and Ş. Ellialtıođlu  
J. Phys.: Condens. Matter **20**, 265003 (2008). [3]

46. "Pt-incorporated anatase  $\text{TiO}_2(001)$  surface for solar cell applications"  
E. Mete, D. Uner, O. Gulseren, Ş. Ellialtıođlu  
Phys. Rev. B **79**, 125418 (2009). [12]
47. "Modification of  $\text{TiO}_2(001)$  surface electronic structure by Au impurity investigated with density functional theory"  
E. Mete, O. Gulseren, and Ş. Ellialtıođlu  
Phys. Rev. B **80**, 035422 (2009). [7]
48. "Dye adsorbates BrPDI, BrGly, and BrAsp on anatase  $\text{TiO}_2(001)$  for dye-sensitized solar cell applications"  
D. Çakır, O. Gulseren, E. Mete, Ş. Ellialtıođlu  
Phys. Rev. B **80**, 035431 (2009). [8]
49. "Atomic and electronic structure of group-IV adsorbates on the GaAs(001)-(1×2) surface"  
D. Usanmaz, M. Cakmak, and Ş. Ellialtıođlu  
Surf. Sci. **603**, 2683 (2009). [2]
50. "Pentacene multilayers on Ag(111) surface"  
E. Mete, I. Demirođlu, M. F. Danisman, and Ş. Ellialtıođlu  
J. Phys. Chem. C **114**, 2724 (2010). [10]
51. "Theoretical analysis of small Pt particles on rutile  $\text{TiO}_2(110)$  surfaces"  
V. Celik, H. Unal, E. Mete, and Ş. Ellialtıođlu  
Phys. Rev. B **82**, 205113 (2010). [10]
52. "Electronic and structural properties of armchair SWCNT/ $\text{TiO}_2(110)$ -(1×2) system"  
C. Tayran, M. Çakmak, and Ş. Ellialtıođlu  
Surf. Sci. **605**, 593 (2011).
53. "Interaction of BrPDI, BrGly, and BrAsp with the Rutile  $\text{TiO}_2(110)$  Surface for Photovoltaic and Photocatalytic Applications: A First-Principles Study"  
D. Çakır, O. Gülseren, E. Mete, and Ş. Ellialtıođlu  
J. Phys. Chem. C **115**, 9220 (2011). [1]
54. "Surface energy and excess charge in (1×2)-reconstructed rutile  $\text{TiO}_2(110)$  from DFT+U calculations"  
Hatice Ünal, Ersen Mete, and Ş. Ellialtıođlu  
Phys. Rev. B **84**, 115407 (2011). [1]
55. "DFT study of noble metal impurities on  $\text{TiO}_2(110)$ "  
E. Mete, O. Gülseren, and Ş. Ellialtıođlu  
Euro. Phys. J. B **85**, 204 (2012).
56. "Influence of steps on the tilting and adsorption dynamics of ordered pentacene films on vicinal Ag(111) surfaces"  
E. Mete, İ. Demirođlu, E. Albayrak, G. Bracco, Ş. Ellialtıođlu, and M. F. Danışman  
J. Phys. Chem. C **116**, 19429 (2012).



## ARTICLES in SCIE :

57. “Raman Scattering and Hall Effect in Layer InSe Under Pressure”  
K. Allakhverdiev, Ş. Ellialtıođlu, A. Ismailov, and Z. Ibragimov  
High Pres. Res. **13**, 121 (1994). [1]
58. “On the structure sensitivity of CO oxidation on alumina supported  
Pd–Pt bi-metallic catalysts”  
S. Kaya, E. Erunal, R. Shaltaf, Ş. Ellialtıođlu, D. Uner  
Turk. J. of Chem. **33**, 11 (2009). [2]

## ARTICLES in WoS :

59. “Phase Transitions in Ternary Layered  $A^3B^3C_2^6$  Group Ferroelectric Semiconductors  
– A Review”  
K. R. Allakhverdiev, T. G. Mamedov, B. G. Akinođlu and Ş. S. Ellialtıođlu  
Turkish J. Phys. **18**, 1–66 (1994). [22]
60. “Enhancement of the Resolution of a Semiconductor Photographic System  
in a Magnetic Field”  
B. G. Salamov, B. G. Akinođlu, Ş. Ellialtıođlu, K. Allakhverdiev,  
and N. N. Lebedeva  
J. Photogr. Sci. **42**, 106 (1994). [21]
61. “Influence of Pressure on the Physical Properties of Chain TlSe-type Crystals”  
K. R. Allakhverdiev and Ş. Ellialtıođlu  
NATO-ARW II-Math, Phys. and Chem. **48**, 119 (2001).  
Eds. H. D. Hochheimer, B. Kuchta, P. K. Dorhout, J. L. Yarger. [4]

Index	Articles	Citations
SCI	56	547
SCIE	2	3
WoS	3	47
Total	61	597
Self		34
Others		563

h-indeks = 13

## **NATIONAL RESEARCH PROJECTS : (+5 BAPs)**

1. “PtSi-Si/CCD Kızılötesi Gözenek Geliştirilmesi”  
DPT/TÜBİTAK [01.07.1992 – 01.10.1994] Yürütücü.
2. “Yüksek Anizotropiye Sahip İkili ve Üçlü Yarıiletkenlerin Fiziksel Özellikleri”  
DPT/TÜBİTAK [01.10.1993 – 01.04.1995] Araştırmacı.
3. “Düşük-Boyutlu Sistemlerin Benzetişimleri, Yapısal ve Elektronik Özellikleri”  
TÜBİTAK [01.01.2002 – 01.01.2004] Yürütücü.
4. “TlSe ve InTe Malzemelerinin Elektronik ve Fononik Özellikleri”  
TÜBİTAK [01.06.2004 – 01.06.2005] Yürütücü.
5. “Titanya Destekli Nanoyapıların ve Yüzeylerin Yapısal ve Elektronik Özellikleri”  
TÜBİTAK [01.10.2007 – 01.10.2010] Yürütücü.
6. “Nano Ölçekli GeSbTe Malzemelerinin Faz-Değişim Mekanizması”  
TÜBİTAK [01.01.2011 – 01.01.2013] Araştırmacı.
7. “Güneş Pili Uygulamaları İçin İlk Prensiplerden Dizayn Edilmiş  
Yüzey Safsızlıklarının Uyarılmış Durum Özellikleri”  
TÜBİTAK [01.10.2010 – 01.10.2013] Araştırmacı.

### **Projects just submitted:**

8. “GaAs(110), GaP(110), ve InP(110) yüzeylerine tutunmuş p ve n tipli  
grafen yapıların elektronik ve kuantum transport özellikleri”  
TÜBİTAK – Yeni Başvuru [2013 – 2016] Araştırmacı.
9. “Altın katalizörler üzerinde alkollerin seçici oksitlenmesi reaksiyon  
mekanizmalarının yük yoğunluğu fonksiyoneli teorisi ile incelenmesi”  
TÜBİTAK – Yeni Başvuru [2013 – 2016] Danışman.

## INVITED TALKS :

1. “ab-initio Calculations of Interstitial Impurities in Metals”  
Ş. Ellialtıođlu  
Dresdener Seminar für Theoretische Physik  
Dresden, DDR, April 15–19, 1985.
2. “Computer Simulation of Growth and Etching”  
Ş. Ellialtıođlu  
2nd General Conference of the Balkan Physical Union  
İzmir, Turkey, September 12–14, 1994.
3. “Computer Simulation of Si and Ge Growth”  
Ş. Ellialtıođlu  
TFD18 (Turkish Physical Society – 18th International Physics Congress)  
Adana, Turkey, September 12–14, 1998.
4. “Electronic Properties of TlSe-type Chain Crystals”  
Ş. Ellialtıođlu  
TFD22 (Turkish Physical Society – 22nd International Physics Congress)  
Bodrum, Turkey, September 14–17, 2004.
5. “Towards theory assisted design of biologically inspired catalysts”  
Ş. Ellialtıođlu  
NANO-TR I NanoScience and NanoTechnology 2005  
Bilkent University, Ankara, Turkey, 25–27 May 2005.
6. “Activation of titania by precious metal incorporation for solar cell applications”  
Ş. Ellialtıođlu  
VI. Renewable Energies Symposium,  
Aegean University, İzmir, Turkey, October 9–11, 2008, pp.36–38.
7. “Understanding and designing highly active titania for photovoltaics  
and photocatalysis by number crunching”  
Ş. Ellialtıođlu  
TFD29 (Turkish Physical Society – 29th International Physics Congress)  
Bodrum, Turkey, September 5–8, 2012.

## INTERNATIONAL CONFERENCES:

### Oral Presentations:

1. “Surface Electronic Properties of d-Band Perovskites”  
Ş. Ellialtıođlu\* and T. Wolfram  
Bull. Am. Phys. Soc. **22**, 315 (1977).  
(APS–March 1977 Meeting, San Diego, California, USA)
2. “Electronic Density of States for the Perovskites”  
T. Wolfram\* and Ş. Ellialtıođlu  
Bull. Am. Phys. Soc. **22**, 410 (1977).  
(APS–March 1977 Meeting, San Diego, California, USA)
3. “Surface Electronic States of d-Band Perovskites”  
Ş. Ellialtıođlu\* and T. Wolfram  
Proc. IV. Rolla Conf. Surface Properties of Materials  
Rolla, Missouri, USA, Aug.1–4, 1977.
4. “Electronic Properties of d-Band Metal Oxides”  
T. Wolfram\* and Ş. Ellialtıođlu  
Midwest Solid State Theory Symposium  
Argonne National Lab., Chicago, Illinois, USA, 1977.
5. “Surface Electronic Properties of d-Band Perovskites”  
Ş. Ellialtıođlu and T. Wolfram\*  
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University of Nebraska, Lincoln, Nebraska, USA, May 13, 1978.
6. “Electronic Structure of Interstitial Impurities in fcc Metals”  
Ş. Ellialtıođlu, H. Akai, R. Zeller and P. H. Dederichs  
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Berlin, FRG, March 18–22, 1985.
7. “Ab-initio Calculations of Interstitial Impurities in Cu”  
Ş. Ellialtıođlu\*, H. Akai, R. Zeller and P. H. Dederichs  
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8. “Surface States and Chemisorption”  
Ş. Ellialtıođlu  
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Bilkent University, Ankara, May 9–13, 1988.
9. “Raman Scattering and Hall Effect Measurements in Layer InSe under Pressure”  
K. R. Allakhverdiev, Ş. Ellialtıođlu\*, A. Ismailov, and I. Ibragimov  
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10. “Phase Transitions in Ternary Mixed System  $Tl(GaSe_2)_x(InS_2)_{1-x}$  Under Pressure”  
K. Allakhverdiev, Ş. Ellialtıođlu\*, T. Fırat, T. Mamedov, and Z. Salaeva  
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pp.145–149.
11. “Monte Carlo Simulations of Pd–Pt Catalysts”  
E. Erunal, Ş. Ellialtıođlu, R. Shaltaf, and D. Uner  
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12. “Effect of molecular structure on the visible light activity of dye sensitizers”  
E. Mete, D. Uner, M. Çakmak, O. Gulseren\*, Ş. Ellialtıođlu  
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13. “Adsorption of BrPDI, BrGly, and BrAsp on Anatase TiO<sub>2</sub>(001) Surface for Dye-sensitized Solar Cell Application”  
D. Çakır, O. Gulseren\*, E. Mete, Ş. Ellialtıođlu , page 20  
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14. “Adsorption of BrPDI, BrGly, and BrAsp dye molecules on rutile TiO<sub>2</sub>(001) surface for Dye-sensitized Solar Cell Application”  
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15. “Activation of rutile TiO<sub>2</sub>(110) by precious metal implantation for solar cell application”  
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16. “Structural investigation of pentacene on Ag(111) by density functional theory”  
M. F. Danisman\*, E. Mete, and Ş. Ellialtıođlu  
APS March09 Meeting, Pittsburgh, Pennsylvania, March 16–20, 2009.
17. “Pentacene multilayers on Ag(111) surface”  
E. Mete\*, I. Demiroglu, M. F. Danisman, Ş. Ellialtıođlu  
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18. “Perylene based dyes on TiO<sub>2</sub> for solar cell applications”  
E. Mete\*, D. Cakir, O. Gulseren, and Ş. Ellialtıođlu  
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19. “DFT calculations towards improved DSSCs”  
Ş. Ellialtıođlu  
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METU, Ankara, November 16–18, 2009.
20. “Electronic and Optical Excitations in Perylene Diimide Derived Dye Molecules from First Principles”  
Kopinjol Baishya\*, Serdar Ögüt, Ersen Mete, Oguz Gülseren, and Şinasi Ellialtıođlu  
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21. “Pentacene thin films on vicinal Ag(111) surfaces”  
M. Fatih Danisman\*, Ersen Mete, Ilker Demiroglu, Şinasi Ellialtıođlu  
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22. “Atomic and electronic structure of stable GeSb<sub>2</sub>Te<sub>4</sub> compound”  
S. Kurt\*, S. Bayram, Ç. Kaderoglu, S. Özkaya, M. Çakmak, B. Alkan, and Ş. Ellialtıođlu  
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Bodrum, September 6–9, 2011.

23. “Interaction of BrPDI, BrGly, and BrAsp with the anatase and rutile TiO<sub>2</sub> surfaces”  
D. Çakir, O. Gülseren\*, E. Mete, Ş. Ellialtıođlu  
ECOSS–28, 28th European Conference on Surface Science  
Wroclaw, Poland, 28 August–2 September 2011.
24. “Electronic structure calculation and analysis of nanosized GeSb<sub>2</sub>Te<sub>4</sub> material”  
S. Kurt\*, S. Bayram, Ç. Kaderoglu, M. Çakmak, B. Alkan, and Ş. Ellialtıođlu  
TFD29, Turkish Physical Society 29th International Physics Congress  
Bodrum, September 5–8, 2012.
25. “Ab initio molecular dynamics study on phase-change materials:  
Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> compound”  
S. Bayram\*, S. Kurt, Ç. Kaderoglu, M. Çakmak, B. Alkan, and Ş. Ellialtıođlu  
TFD29, Turkish Physical Society 29th International Physics Congress  
Bodrum, September 5–8, 2012.

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### Poster Presentations:

1. “An Investigation of the Interface Electronic Structure of Si–SiO<sub>2</sub> Junctions”  
S. Çıracı, Ş. Ellialtıođlu and Ş. Erkoç  
PCSI 9 Proc. MS# 901–24 Asilomar, California, USA, Feb. 1982.
2. “STM Line Scans” Ş. Ellialtıođlu and S. Çıracı  
7th General Conference, Condensed Matter Division of EPS  
Pisa, Italy, April 7–10, 1987.
3. “Electronic Structure of Strained Si<sub>n</sub>/Ge<sub>n</sub>(001) Superlattices”  
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5. “Bandgap Modulation of GaSe Type Semiconductors by Coherently Excited Raman Active Optical Phonons”  
K. Allakhverdiev and Ş. Ellialtıođlu  
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6. “Electronic Properties of Ge and Si Quantum Wires”  
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7. “Electronic Properties of High Indexed Germanium Surfaces”  
Şinasi Ellialtıođlu  
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8. “Ab initio study of the adsorption and desorption of Se on the Si(001) surface”  
M. Çakmak, G. P. Srivastava, Ş. Ellialtıođlu, and K. Çolakođlu  
ECOSS–20 (20th European Conference on Surface Science)  
Krakow, Poland, Sept. 4–7, 2001.
9. “Simulation of amorphous and crystalline growth of tetrahedral semiconductors”  
R. Shaltaf and Ş. Ellialtıođlu  
ECOSS–20 (20th European Conference on Surface Science)  
Krakow, Poland, Sept. 4–7, 2001.
10. “Ab initio study of the one-monolayer Sb/Si(001) interface”  
M. Çakmak, R. Shaltaf, G. P. Srivastava, and Ş. Ellialtıođlu  
ECOSS–21 (21st European Conference on Surface Science)  
NANO-7 (7th Int. Conf. on Nanometer-Scale Science and Technology)  
Malmö, Sweden, June 24–28 2002.

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R. Shaltaf, M. Çakmak, E. Mete, G. P. Srivastava, Ş. Ellialtıođlu  
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Praha, Czech Republic, Sept. 7–12, 2003.
12. “An ab initio study of the Te surfactant on Ge/Si(001)”  
M. Çakmak, G. P. Srivastava, and Ş. Ellialtıođlu  
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13. “Ab initio study of Bi surfactant on Ge/Si(001) surface”  
M. Çakmak, G. P. Srivastava, and Ş. Ellialtıođlu  
IVC–16 (16th International Vacuum Congress)  
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NANO–8 (8th Int. Conf. on Nanometer-Scale Science and Technology)  
Venice, Italy, June 28–July 2, 2004.
14. “Activity and structure predictions on mono and bimetallic  
precious metal catalysts”  
E. Erunal, Ş. Ellialtıođlu, R. Shaltaf, and D. Uner,  
EUROPACAT-VII, August 28–September 1, 2005 Sofia, Bulgaria.
15. “Tailoring the Structures of the Organic Dyes for Enhanced Electron Transfer  
Processes during the Photoreduction of CO<sub>2</sub> on a TiO<sub>2</sub> Surface”  
F. Yukruk, O. Ozcan, E. Mete, E. U. Akkaya, D. Uner, M. Cakmak, O. Gulseren,  
and Ş. Ellialtıođlu  
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16. “Estimating the electron transfer efficiencies from organic dyes to  
Pt-promoted TiO<sub>2</sub> structures during the gas phase photoreduction of CO<sub>2</sub>”  
O. Ozcan, F. Yukruk, E. Mete, E. U. Akkaya, D. Uner, M. Cakmak, O. Gulseren,  
and Ş. Ellialtıođlu  
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17. “Atomic and electronic structures of Sr/Si(001)-2×2”  
M. Cakmak, E. Mete, and Ş. Ellialtıođlu  
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19. “Adsorption and photocatalytic activity of perylene-diimide based  
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O. Gulseren, E. Mete, D. Uner, and Ş. Ellialtıođlu  
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21. “Effect of hydrogenation on B/Si(001)-(1×2)”  
M. Cakmak, E. Mete, and Ş. Ellialtıođlu  
ECOSS–24, Paris, France, 4–8 September 2006.  
(24th European Conference On Surface Science).
  22. “An ab initio study of 3-aminopropyltrimetoxysilane molecule  
on Si(111)-( $\sqrt{3} \times \sqrt{3}$ )R30°”  
G. Demirel, M. Cakmak, T. Caykara, and Ş. Ellialtıođlu  
ECOSS–24, Paris, France, 4–8 September 2006.  
(24th European Conference On Surface Science).
  23. “Atomic and electronic structures of Bi/InP(001)- $\alpha$ 2(2×4)”  
D. Usanmaz, M. Çakmak\*, and Ş. Ellialtıođlu  
IVC-17/ICSS-13 ve ICN+T2007 (ve NCSS-6/NSM-22/SVM-4),  
Stockholm, Sweden, 2–6 July 2007.
  24. “Electronic structure of Au-implanted TiO<sub>2</sub> surfaces”  
E. Mete, M. Çakmak, O. Gulseren\*, Ş. Ellialtıođlu  
NANO–TR IV, Istanbul Technical University, Istanbul, 9–13 June 2008.
  25. “Adsorption of BrPDI, BrGly, and BrAsp on Anatase TiO<sub>2</sub>(001) Surface  
for Dye-sensitized Solar Cell Application”  
D. Çakır, O. Gulseren\*, E. Mete, Ş. Ellialtıođlu  
NANO–TR IV, Istanbul Technical University, Istanbul, 9–13 June 2008.
  26. “Electronic structure of Au-implanted TiO<sub>2</sub> surfaces”  
E. Mete, M. Çakmak, O. Gulseren\*, Ş. Ellialtıođlu  
ECOSS25, Liverpool, UK, 28 July–1 August 2008.
  27. “Adsorption of BrPDI, BrGly, and BrAsp on Anatase TiO<sub>2</sub>(001) Surface  
for Dye-sensitized Solar Cell Application”  
D. Çakır, O. Gulseren\*, E. Mete, Ş. Ellialtıođlu  
ECOSS–25, Liverpool, UK, 28 July–1 August 2008.
  28. “Structural and electronic properties of carbon nanotubes  
on the rutile TiO<sub>2</sub>(110)-(1×2) surface”  
C. Tayran, M. Çakmak, E. Mete, and Ş. Ellialtıođlu  
TFD25, Bodrum, 25–29 August 2008.
  29. “Atomic structures of group-IV on GaAs(001)-(1×2) surfaces”  
D. Usanmaz, M. Çakmak, and Ş. Ellialtıođlu  
TFD25, Bodrum, 25–29 August 2008.
  30. “A Computational Study of Pentacene Thin Films on Ag(111) Surface”  
E. Mete, I. Demiroglu, M. F. Danisman\*, and Ş. Ellialtıođlu  
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  31. “Electronic properties of carbon nanotubes adsorbed on reconstructed  
rutile TiO<sub>2</sub>(110)-1×2 surface”  
C. Tayran\*, M. Çakmak, and Ş. Ellialtıođlu  
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32. “Electronic properties of carbon nanotubes adsorbed on reconstructed rutile  $\text{TiO}_2(110)$  surface: A DFT study”  
Ceren Tayran\*, Mehmet Cakmak, and Şinasi Ellialtıođlu  
ECOSS–26, Parma, Italy, August 30–Sept 4, 2009.
33. “Structural and Electronic Investigation of Pentacene Thin Films on Flat and Stepped  $\text{Ag}(111)$  Surfaces”  
M. F. Danisman, E. Mete, B. Özkan, I. Demirođlu, Ş. Ellialtıođlu  
NANO–TR VI, İzmir Yüksek Teknolođi Enstitüsü, İzmir, 2010.
34. “Small Pt particles on rutile  $\text{TiO}_2(110)$ ”  
E. Mete, V. Celik, and Ş. Ellialtıođlu  
ECOSS27 Groningen, Holland, August 29–Sept. 3, 2010.
35. “Armchair double-walled carbon nanotube on rutile  $\text{TiO}_2(110)-(1\times 2)$ ”  
C. Tayran, M. Cakmak, and Ş. Ellialtıođlu  
17th International Conference on Ternary and Multinary Compounds  
ICTMC–17 Sept. 28–30, Baku, 2010.
36. “Pentacene thin films on vicinal  $\text{Ag}(111)$  surfaces”  
M. Fatih Danisman, Ersen Mete, Ilker Demirođlu, Şinasi Ellialtıođlu  
241st ACS National Meeting, 27–31 March, 2011 Anaheim, CA.
37. “Adsorption of Gold–Copper Metal Alloys on Anatase  $\text{TiO}_2(100)$  Surface”  
K. B. Vural, E. Mete, and Ş. Ellialtıođlu  
TFD28, Turkish Physical Society 28th International Physics Congress  
Bodrum, September 6–9, 2011.
38. “Electronic structure of phase-change materials  $\text{GeSb}_2\text{Te}_4$  and  $\text{Ge}_2\text{Sb}_2\text{Te}_5$  :  
An ab-initio calculation”  
S. Kurt, S. Bayram, Ç. Kaderođlu, S. Özkaya, M. Çakmak, B. Alkan,  
and Ş. Ellialtıođlu  
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San Francisco, CA, April 9–13, 2012.

## NATIONAL CONFERENCES :

### Oral Presentations:

1. "Electronic Properties of Vacancies in Si and SiO<sub>2</sub> Crystals"  
Ş. Erkoç\*, S. Çıracı, Ş. Ellialtıođlu and M. Tomak  
TÜBİTAK–Solid State Physics Unit–Colloquium II  
(METU, Ankara, Feb. 1982), pp. 23–25.
2. "Electronic Energy Spectrum of Oxygen Chemisorbed Silicon Surfaces"  
Ş. Ellialtıođlu\*, S. Çıracı and Ş. Erkoç  
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3. "Interface Electronic Structure of Si–SiO<sub>2</sub> Junctions"  
S. Çıracı\*, Ş. Ellialtıođlu and Ş. Erkoç  
TÜBİTAK–Solid State Physics Unit–Colloquium II  
(METU, Ankara, Feb. 1982), pp. 29–31.
4. "Amorf Silisyum Üzerine Çalışmalar"  
M. C. Yalabık\* and Ş. Ellialtıođlu  
1st Ankara Conference on Condensed Matter Physics  
(Hacettepe University, Ankara, 1984).
5. "Computer Simulation of the Structure of Amorphous Silicon  
using Monte–Carlo Technique"  
G. Dereli\*, Ş. Ellialtıođlu and M. C. Yalabık  
Bilgisayar Benzetişim Yöntemlerinin Fizik ve Mekanik Problemlerine  
Uygulanması Sempozyumu (Symposium on the Applications of  
Computer Simulation Techniques on Physics and Mechanics Problems)  
Eds. Y. Gündüç ve A. Hacınlıyan  
(Boğaziçi Üniversitesi, İstanbul, Ocak 1987) pp. 30–49.
6. "Adatom Chemisorption on Perovskite Surfaces"  
H. Kökten\* and Ş. Ellialtıođlu  
I. National Condensed Matter Physics Congress  
Turkish Physical Association, Bodrum, September 27–29, 1988, p.19.
7. "Electronic Structure of Si and Ge Quantum Wires"  
Ş. Ellialtıođlu  
5th Ankara Conference on Condensed Matter Physics  
(METU, Ankara, 1997).
8. "a-Ge büyütmesi benzetişimi"  
G. Oylumluođlu\*, Ş. Oktik, ve Ş. Ellialtıođlu  
Boğaziçi Üniversitesi, Kimyasal Fizik Toplantısı, 1998.
9. "Monte Carlo Simulation of Amorphous Germanium"  
Ş. Ellialtıođlu\*, G. Oylumluođlu and Ş. Oktik  
6th Ankara Conference on Condensed Matter Physics  
(Bilkent University, Ankara, 1998).
10. "a-Ge büyütmesi benzetişimi"  
G. Oylumluođlu\*, Ş. Oktik, ve Ş. Ellialtıođlu  
TFD XV Kongresi, (Çukurova University, Adana 1999).

11. "Electronic Properties of Relaxed Ge(113) Surface"  
Ş. Ellialtıođlu\* and R. Shaltaf  
TFD XV Kongresi, (Çukurova University, Adana 1999).
12. "A Study of Mg Adsorption On Si(001) Surface From First Principles"  
R. Shaltaf\*, E. Mete, Ş. Ellialtıođlu  
10.ncu Yođun Madde Fiziđi – Ankara Toplantısı,  
Hacettepe Üniversitesi, Ankara, 14 Kasım 2003.
13. "Bir 4d-perovskitin Elektronik ve Yapısal Özellikleri: SrZrO<sub>3</sub>'in Kübik Fazı"  
E. Mete\*, R. Shaltaf, Ş. Ellialtıođlu  
10.ncu Yođun Madde Fiziđi – Ankara Toplantısı,  
Hacettepe Üniversitesi, Ankara, 14 Kasım 2003.
14. "Energy Bands of TlSe and TlInSe<sub>2</sub> in Tight Binding Model"  
E. Mete\*, Ö. Yıldırım, and Ş. Ellialtıođlu  
12.nci Yođun Madde Fiziđi – Ankara Toplantısı,  
Ankara Üniversitesi, Fen Fakültesi Ankara, 18 Kasım 2005.
15. "Bimetalik Pd–Pt katalizörlerinde Monte Carlo yöntemi ile yüzey yapısı hesaplamaları"  
E. Erunal\*, Ş. Ellialtıođlu, R. Shaltaf, and D. Uner  
UMMK7 (Eskişehir, Anadolu Üniversitesi 2006).
16. "Pt<sub>n</sub> (n=1–4) topaklarının stokiyometrik ve indirgenmiş rutil TiO<sub>2</sub>(110) yüzeylerinde büyüme eğilimi"  
E. Mete\* ve Ş. Ellialtıođlu  
13.ncü Yođun Madde Fiziđi – Ankara Toplantısı,  
Orta Dođu Teknik Üniversitesi, Ankara, 3 Kasım 2006.
17. "ABO<sub>3</sub> yapılı geçiş-metal oksitlerin elektronik özellikleri"  
Ş. Ellialtıođlu (Colloquium)  
İstanbul Teknik Üniversitesi, İstanbul, 23 Mart 2007.
18. "Ag(111) yüzeylerinde düzenli pentasen tabakaları"  
E. Mete\*, İ. Demirođlu, M. F. Danisman, Ş. Ellialtıođlu  
16.ncı Yođun Madde Fiziđi – Ankara Toplantısı,  
Gazi Üniversitesi, Ankara, 6 Kasım 2009.
19. "Rutil TiO<sub>2</sub>(110)-(1×2) Yüzeyine Koltuk Tipi Tek-Duvarlı GaN Nanotüplerin Tutunması"  
N. Akın\*, M. Çakmak, ve Ş. Ellialtıođlu  
NABITEK 2010, 20–23 Haziran 2010, İstanbul.
20. "Küçük Pt parçacıklarının rutil TiO<sub>2</sub>(110) yüzeylerinde LSDA+U tasviri  
Ersen Mete\*, Veysel Çelik, Hatice Ünal, ve Şinasi Ellialtıođlu  
17.nci Yođun Madde Fiziđi – Ankara Toplantısı,  
Ankara Üniversitesi, Ankara, 5 Kasım 2010.
21. "TiO<sub>2</sub>(110) yüzeyinde güneş pili uygulamaları için oluşturulmuş kusur durumlarının analizi"  
V. Çelik\*, H. Ünal, E. Mete, ve Ş. Ellialtıođlu  
18.nci Yođun Madde Fiziđi – Ankara Toplantısı,  
ODTÜ, 25 Kasım 2011, Sayfa S05.

## NATIONAL CONFERENCES :

### Poster Presentations:

1. "Theoretical and Experimental Studies on CO Oxidation over Pt–Pd Bimetallic Catalysts"  
E. Erunal, S. Kaya, R. Shaltaf, Ş. Ellialtıođlu, and Deniz Uner  
NCC-1: First National Catalysis Conference  
METU NCC, Guzelyurt, NC, 17–20 January 2007.
2. "X/GaAs(001)-(1×2) yüzeyinin atomik ve elektronik özellikleri: (X = C, Ge, Sn)"  
D. Usanmaz, M. Çakmak, ve Ş. Ellialtıođlu  
15.nci Yođun Madde Fiziđi – Ankara Toplantısı,  
Bilkent Üniversitesi, Ankara, 7 Kasım 2008.
3. "Rutil TiO<sub>2</sub>(110)-(1×2) yüzeti üzerindeki Karbon Nanotüp'ün yapısal ve elektronik özellikleri"  
C. Tayran, M. Çakmak, E. Mete, ve Ş. Ellialtıođlu  
15.nci Yođun Madde Fiziđi – Ankara Toplantısı,  
Bilkent Üniversitesi, Ankara, 7 Kasım 2008.
4. "Altın Öbeklerinin Anataz TiO<sub>2</sub>(100),(001), ve (101) yüzeylerine bağlanması"  
K. B. Vural, E. Mete, ve Ş. Ellialtıođlu  
15.nci Yođun Madde Fiziđi – Ankara Toplantısı,  
Bilkent Üniversitesi, Ankara, 7 Kasım 2008.
5. "Rutil TiO<sub>2</sub>(110) yüzeylerinde SO<sub>2</sub> tutunması"  
M. Mesta, E. Mete, ve Ş. Ellialtıođlu  
15.nci Yođun Madde Fiziđi – Ankara Toplantısı,  
Bilkent Üniversitesi, Ankara, 7 Kasım 2008.
6. "TiO<sub>2</sub> destekli nanoyapıların ve yüzeylerin yapısal ve elektronik özellikleri"  
N. Akin, M. Çakmak, ve Ş. Ellialtıođlu  
16.ncı Yođun Madde Fiziđi – Ankara Toplantısı,  
Gazi Üniversitesi, Ankara, 6 Kasım 2009.
7. "Rutil TiO<sub>2</sub>(110)-(1×2) yüzeyine tutunmuş karbon nanotüpün elektronik özellikleri"  
C. Tayran, M. Çakmak, ve Ş. Ellialtıođlu  
16.ncı Yođun Madde Fiziđi – Ankara Toplantısı,  
Gazi Üniversitesi, Ankara, 6 Kasım 2009.
8. "BN Nanotüpün TiO<sub>2</sub> Yüzeyine Tutunması: Yapısal ve Elektronik Özellikler"  
M. Biçen, M. Çakmak, ve Ş. Ellialtıođlu  
NABITEK 2010, 20–23 Haziran 2010, İstanbul.
9. "TiO<sub>2</sub>(110) rekonstrüksiyon modellerinin DFT+*U* analizi"  
Hatice Ünal, Veysel Çelik, Ersen Mete, ve Şinasi Ellialtıođlu  
17.nci Yođun Madde Fiziđi – Ankara Toplantısı,  
Ankara Üniversitesi, Ankara, 5 Kasım 2010.
10. "Rutil TiO<sub>2</sub>(110)-(1×2) Yüzeyine GaN Nanotüp Tutunmasının Atomik ve Elektronik Özelliklerinin İncelenmesi"  
Nihan Akin, Mehmet Çakmak, ve Şinasi Ellialtıođlu  
17.nci Yođun Madde Fiziđi – Ankara Toplantısı,  
Ankara Üniversitesi, Ankara, 5 Kasım 2010.

11. "BN Nanotüpün TiO<sub>2</sub> Yüzeyine Tutunması: Yapısal ve Elektronik Özellikler  
M. Biçen, M. Çakmak, ve Ş. Ellialtıođlu  
17.nci Yođun Madde Fiziđi – Ankara Toplantısı,  
Ankara Üniversitesi, Ankara, 5 Kasım 2010.

## THESES GIVEN

1. “Charge Asymmetry and a Theoretical Prediction of n–n Scattering Length”  
M.S. Degree, 1973, Middle East Technical University, Ankara, Turkey.  
(Prof. Dr. C. Yalçın).
2. “Electronic Properties of d-Band Perovskites”  
Ph.D. Degree, 1977, University of Missouri–Columbia, Columbia, MO, USA.  
(Prof. Tom Wolfram).
3. “Electronic Properties of Defect States on d-Band Metal-Oxides  
and Chemisorption”  
Habilitation Thesis (Dozentship), 1982.

## Ph.D. THESES SUPERVISED

1. “Computer Simulation of the Structure of Amorphous Silicon  
using Monte–Carlo Technique”  
Gülây Dereli, June 1987.
2. “Two-Dimensional Systems in Solid State Physics”  
Şenay Katırcıoğlu, December 1987.  
(principal advisor: Prof. Dr. Salim Çıracı).
3. “A Tight-Binding Model of Chemisorption on Perovskite Surfaces”  
Hatice Kökten, January 1993.
4. “Electronic Properties of Transition Metal Oxides”  
Ersen Mete, December 2003.
5. “Adsorption and Growth on Si(001) Surface”  
Riad Shaltaf, April 2004.
6. “Steady State and Transient Simulations in 2D and 3D for Crystal Growth  
by Vertical Bridgman Systems”  
Ergun Taşarkuyu, January 2003.  
(principal advisor: Doç. Dr. Bülent Akınoğlu).
7. “The Structure, Energetics and Melting Behavior of Free Platinum Clusters”  
Ali Sebetci, January 2004 (co-advisor).

### Thesis in progress:

8. “Adsorption of metal atoms on anatase TiO<sub>2</sub> surfaces”  
Kıvılcım Başak Vural, expected graduation date: December 2014.

## M.S. THESES SUPERVISED

1. “Jellium Calculations for Metallic Slabs”  
Bassam Daghlas, September 1987.
2. “Construction of a Scanning Tunneling Microscope and its Application to Graphite Surface in Air”  
İsmet İnönü Kaya, February 1990.  
(principal-advisor: Prof. Dr. Recai Ellialtıođlu).
3. “On the Theory of Conventional and High  $T_c$  Superconductivity”  
Ali Serdar Öđüt, June 1990.
4. “Amorf Germanyumun Büyütülmesinin Monte Carlo Simülasyonu”  
Görkem Oylumluođlu, September 1999.  
(co-advisor: Prof. Dr. Şener Oktik).
5. “Energy Bands of TlSe and TlInSe<sub>2</sub> in Tight Binding Model”  
Özlem Yıldırım, September 2005.
6. “Structure Sensitivity of Selective CO Oxidation over Precious Metal Catalysts”  
Bora Atalık, February 2005.  
(principal advisor: Prof. Dr. Deniz Üner).
7. “Structure and activity predictions on supported mono- and bi-metallic catalysts”  
Ebru Erünal, April 2006.  
(principal advisor: Prof. Dr. Deniz Üner).
8. “Electronic Properties of Dye Molecules Adsorbed on Anatase-Titania Surface for Solar Cell Applications”  
Engin Torun, August 2009.  
(principal advisor: Doç. Dr. Hande Toffoli).
9. “Adsorption of Aromatic Molecules on Rutile TiO<sub>2</sub>(110) Surfaces”  
Murat Mesta, September 2009.
10. “Adsorption of Gold Atoms on Anatase TiO<sub>2</sub>(100)-1×1 Surface”  
Kıvılcım Başak Vural, September 2009.
11. “Density Functional Theory Investigation of TiO<sub>2</sub> Anatase Nanosheets”  
Sibel Ceren Sayın, September 2009.  
(principal advisor: Doç. Dr. Hande Toffoli).
12. “Ab-initio studies of pentacene on Ag(111) surfaces”  
İlker Demirođlu, January 2010.  
(principal advisor: Doç. Dr. Mehmet Fatih Danıřman).

### **Thesis in progress:**

13. “Investigation of atomic and electronic structure of ternary (GeTe)<sub>m</sub>(SbTe)<sub>n</sub> (GST) phase-change materials”  
Sibel Kurt Homurlu, expected graduation date:December 2013.



**The Courses Given at METU:**

- Phys 105–106 General Physics I–II
- Phys 202 Modern Physics
- Phys 215 Advanced Modern Physics
- Phys 291 Properties of Materials for EE
- Phys 309–310 Introduction to Solid State Physics I–II
- Phys 312 Solid State Physics
- Phys 303–304 Quantum Theory and its Applications I–II
- Phys 321–322 Quantum Physics I–II
- Phys 331–332 Electromagnetic Theory I–II
- Phys 431 Quantum Mechanics I
- Phys 400 Graduation Project
- Phys 415–416 Projects in Physics I–II
- Phys 409–410 Condensed Matter Physics I–II
- Phys 515–516 Special Topics in Solid State Physics I–II
- Phys 531–532 Solid State Theory I–II
- Phys 558–559 Topics in Theoretical Physics I–II
- Phys 565 Topics in Mathematical Physics I

**The Courses Given at Konya Selçuk Üniversitesi (1978–1981) :**

- Fiz 101–102 Genel Fizik I–II
- Fiz 612 Yarı İletkenler Fiziği

**The Courses Given at Bilkent University (1987–1988) :**

- Phys 301–302 Introduction to Condensed Matter Physics I–II

**The Course Given at Georgia Institute of Technology (1996) :**

- Phys 102 General Physics II

**The Course Given at TED University (2012) :**

- Phys 101 General Physics I