

## Personal Information

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## Advising Theses

- ÖNAL I., Quantum mechanical study of propylene epoxidation on various metal oxide surfaces, Doctorate, İ.TEZSEVİN(Student), 2018
- ÖNAL I., Theoretical and experimental investigation of water-gas shift reaction over supported copper/iron oxide catalysts, Doctorate, Ö.YALÇIN(Student), 2017
- ÖNAL I., Quantum mechanical investigation of CO oxidation conducted on automotive exhaust emission catalysts containing La and Pd/La on ceria-zirconia, Post Graduate, Y.KAYA(Student), 2016
- ÖNAL I., Propylene epoxidation on CuO and Li promoted cuo catalysts: A density functional theory study, Post Graduate, M.GEZER(Student), 2014
- ÖNAL I., Development of three way catalytic converters for elimination of hydrocarbons, carbon monoxide and nitric oxide in automotive exhaust, Post Graduate, A.CİVAN(Student), 2014
- ÖNAL I., Exhaust gas cleaning by three way catalytic converters, Post Graduate, Z.KARAKOÇ(Student), 2013
- ÖNAL I., Removal of hydrocarbons, carbon monoxide and nitric oxides in automotive exhaust with three way catalytic converter, Post Graduate, D.GERÇEKER(Student), 2013
- ÖNAL I., Catalytic reaction of propylene to propylene oxide on various catalysts, Post Graduate, Ş.KALYONCU(Student), 2012
- ÖNAL I., Application of density functional theory to propylene to propylene oxide catalytic reaction, Post Graduate, D.ONAY(Student), 2012
- ÖNAL I., A study of catalytic nanocarbon synthesis by means of quantum mechanical methods, Post Graduate, İ.TEZSEVİN(Student), 2012
- ÖNAL I., Computational study of ethylene epoxidation, Doctorate, M.OLUŞ(Student), 2011
- ÖNAL I., Epoxidation reactions of small alkenes on catalytic surfaces, Post Graduate, E.KURNAZ(Student), 2011
- ÖNAL I., A quantum chemical study of water and ammonia adsorption mechanisms on titanium dioxide surfaces, Post Graduate, R.ERDOĞAN(Student), 2010
- ÖNAL I., A DFT study of ethylene adsorption and hydrogenation mechanisms on nickel, Post Graduate, N.DUYGU(Student), 2010
- ÖNAL I., Development of sol-gel catalysts by use of fast combinatorial synthesis and high throughput testing techniques for catalytic oxidation of propylene to propylene oxide, Doctorate, D.DÜZENLİ(Student), 2010
- ÖNAL I., Catalytic partial oxidation of propylene on metal surfaces by means of quantum chemical methods, Post Graduate, A.CAN(Student), 2010
- ÖNAL I., Development of a three way catalytic converter for elimination of hydrocarbons, carbon monoxide and nitric oxide in automotive exhaust, Post Graduate, N.KANDİLLİ(Student), 2010
- ERKOÇ Ş., ÖNAL I., Quantum mechanical treatment of fullerene-based systems doped with various metal and non-metal elements as prospective spin-qubits, Post Graduate, S.POLAD(Student), 2010
- ÖNAL I., A density functional theory study of catalytic epoxidation of ethylene and propylene, Doctorate, M.FERDİ(Student), 2009
- ÖNAL I., Quantum mechanical calculation of nitrous oxide decomposition on transition metals, Post Graduate, M.KAAN(Student), 2007
- ÖNAL I., Quantum chemical simulation of nitric oxide reduction by ammonia (SCR reaction) on V2O5/TiO2 catalyst surface, Post Graduate, S.SOYER(Student), 2005
- ÖNAL I., Quantum mechanical calculation of ethylene hydrogenation on nickel 111 single crystal surface and nickel nanoclusters, Post Graduate, A.SAYAR(Student), 2005
- ÖNAL I., Quantum chemical simulation of NO reduction by ammonia (SCR reaction) on V2O5 catalyst surface, Post Graduate, A.UZUN(Student), 2003
- ÖNAL I., Catalytic partial oxidation of methane to formaldehyde, Post Graduate, B.AKBULUT(Student), 2000
- ÖNAL I., Computational quantum chemical study of oxidative dehydrogenation of propene to propylene, Post Graduate,

N.UZMAN(Student), 2000

ÖNAL I., Catalytic partial oxidation of methane, Doctorate, Ş.ÖZTÜRK(Student), 1998

ÖNAL I., An Investigation on the production of sialon ceramics by sol-gel method, Post Graduate, C.AKSEL(Student), 1996

DOĞU T., ÖNAL I., Oxidative coupling of methane using superconductor and semiconductor type catalytic materials, Doctorate, Y.ERARSLANOĞLU(Student), 1995

ÖNAL I., The Use of natural zeolite as catalyst in the production of ethylbenzene, Post Graduate, Ö.ESEN(Student), 1994

ÖNAL I., Production of sialon ceramics via sol-gel process, Post Graduate, M.NİLGÜN(Student), 1992

ÖNAL I., Efficient catalysts for oxidative coupling of methane, Post Graduate, O.ALTIN(Student), 1992

ÖNAL I., Transient modeling of diffusivity for monolithic catalyst by using pulse testing technique, Post Graduate, Z.KHEDR(Student), 1991

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

- **Role of Local Structure on Catalytic Reactivity: Comparison of Methanol Oxidation by Aqueous Bioinorganic Enzyme Mimic (Vanadium Haloperoxidase) and Vanadia-Based Heterogeneous Catalyst (Supported VO<sub>4</sub>/SiO<sub>2</sub>)**  
Yalcin O., Erwin J. E. M., Gerceker D., ÖNAL I., Wachs I. E.  
ACS CATALYSIS, vol.10, pp.1566-1574, 2020 (Journal Indexed in SCI)
- **A comparative experimental and density functional study of glucose adsorption and electrooxidation on the Au-graphene and Pt-graphene electrodes**  
Caglar A., Duzenli D., ÖNAL I., Tersevin I., Sahin O., Demir Kıvrak H.  
INTERNATIONAL JOURNAL OF HYDROGEN ENERGY, vol.45, pp.490-500, 2020 (Journal Indexed in SCI)
- **A density functional theory study of propylene epoxidation mechanism on Ag<sub>2</sub>O(001) surface**  
Tezsevin I., van Santen R. A., ÖNAL I.  
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, vol.20, pp.26681-26687, 2018 (Journal Indexed in SCI)
- **Density functional theory study of interactions between carbon dioxide and functionalized polyhedral oligomeric silsesquioxanes**  
Tezsevin I., Demirtas C., ÖNAL I., DİLEK HACIHABİBOĞLU Ç.  
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, vol.117, 2017 (Journal Indexed in SCI)
- **A density functional theory study of propylene epoxidation on RuO<sub>2</sub>(110) surface**  
Atmaca D. O., Duzenli D., Ozbek M. O., ÖNAL I.  
APPLIED SURFACE SCIENCE, vol.385, pp.99-105, 2016 (Journal Indexed in SCI)
- **Theoretical and experimental investigation of water gas shift (WGS) reaction over iron oxide catalysts**  
Yalcin O., ÖNAL I., Wachs I.  
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, vol.252, 2016 (Journal Indexed in SCI)
- **A density functional theory study of partial oxidation of propylene on Cu<sub>2</sub>O(001) and CuO(001) surfaces**  
Duzenli D., Atmaca D. O., Gezer M. G., ÖNAL I.  
APPLIED SURFACE SCIENCE, vol.355, pp.660-666, 2015 (Journal Indexed in SCI)
- **A Density Functional Theory Study of NO Reduction by C<sub>3</sub>H<sub>8</sub> Aided Selective Catalytic Reduction Method**  
Tezsevin I., Onay D., FELLAH M. F., ÖNAL I.  
CATALYSIS LETTERS, vol.145, pp.964-970, 2015 (Journal Indexed in SCI)
- **Direct epoxidation of propylene to propylene oxide on various catalytic systems: A combinatorial micro-reactor study**  
Kalyoncu S., Duzenli D., ÖNAL I., Seubsai A., Noon D., Senkan S.  
CATALYSIS COMMUNICATIONS, vol.61, pp.16-20, 2015 (Journal Indexed in SCI)
- **NaCl-Promoted CuO-RuO<sub>2</sub>/SiO<sub>2</sub> Catalysts for Propylene Epoxidation with O<sub>2</sub> at Atmospheric Pressures: A Combinatorial Micro-reactor Study**  
Kalyoncu S., Duzenli D., ÖNAL I., Seubsai A., Noon D., Senkan S., Say Z., Vovk E. I., ÖZENSOYE.  
CATALYSIS LETTERS, vol.145, pp.596-605, 2015 (Journal Indexed in SCI)
- **DFT investigation of high temperature water gas shift reaction on chromium-iron mixed oxide catalyst**

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INTERNATIONAL JOURNAL OF HYDROGEN ENERGY, vol.39, pp.19563-19569, 2014 (Journal Indexed in SCI)

- **A DFT study on CO oxidation on Pd-4 and Rh-4 clusters and adsorbed Pd and Rh atoms on CeO<sub>2</sub> and Ce(0.75)Zr(0.25)O(2) supports for TWC applications**

Gerceker D., ÖNAL I.

APPLIED SURFACE SCIENCE, vol.285, pp.927-936, 2013 (Journal Indexed in SCI)

- **Density functional theory investigation of acetylene dehydrogenation on metal exchanged ZSM-5 clusters for initial step of carbon nanotube production**

Tezsevin I., FELLAH M. F. , ÖNAL I.

MICROPOROUS AND MESOPOROUS MATERIALS, vol.180, pp.102-108, 2013 (Journal Indexed in SCI)

- **A DFT Study of Ethylene Hydrogenation Reaction Mechanisms on Ni-13 Nanocluster**

Yilmazer N. D. , FELLAH M. F. , ÖNAL I.

TOPICS IN CATALYSIS, vol.56, pp.789-793, 2013 (Journal Indexed in SCI)

- **Chlorine and Caesium Promotion of Silver Ethylene Epoxidation Catalysts**

Ozbek M. O. , ÖNAL I., van Santen R. A.

CHEMCATCHEM, vol.5, pp.443-451, 2013 (Journal Indexed in SCI)

- **A DFT study on the [VO](1+)-ZSM-5 cluster: direct methanol oxidation to formaldehyde by N<sub>2</sub>O**

FELLAH M. F. , ÖNAL I.

PHYSICAL CHEMISTRY CHEMICAL PHYSICS, vol.15, pp.13969-13977, 2013 (Journal Indexed in SCI)

- **Epoxidation of Propene by High-Throughput Screening Method Over Combinatorially Prepared Cu Catalysts Supported on High and Low Surface Area Silica**

Duzenli D., ŞEKER E., Senkan S., ÖNAL I.

CATALYSIS LETTERS, vol.142, pp.1234-1243, 2012 (Journal Indexed in SCI)

- **Effect of Surface and Oxygen Coverage on Ethylene Epoxidation**

Ozbek M. O. , ÖNAL I., van Santen R. A.

TOPICS IN CATALYSIS, vol.55, pp.710-717, 2012 (Journal Indexed in SCI)

- **Epoxidation of Propylene on a [Ag<sub>14</sub>O<sub>9</sub>] Cluster Representing Ag<sub>2</sub>O (001) Surface: A Density Functional Theory Study**

Fellah M. F. , ÖNAL I.

CATALYSIS LETTERS, vol.142, pp.22-31, 2012 (Journal Indexed in SCI)

- **Ni-55 nanocluster: a density functional theory study of the binding energy of nickel and ethylene adsorption**

Yilmazer N. D. , Fellah M. F. , ÖNAL I.

TURKISH JOURNAL OF CHEMISTRY, vol.36, pp.55-67, 2012 (Journal Indexed in SCI)

- **Why silver is the unique catalyst for ethylene epoxidation**

Ozbek M. O. , ÖNAL I., van Santen R. A.

JOURNAL OF CATALYSIS, vol.284, pp.230-235, 2011 (Journal Indexed in SCI)

- **Ethylene epoxidation catalyzed by chlorine-promoted silver oxide**

Ozbek M. O. , ÖNAL I., Van Santen R. A.

JOURNAL OF PHYSICS-CONDENSED MATTER, vol.23, 2011 (Journal Indexed in SCI)

- **C-H bond activation of methane on M- and MO-ZSM-5 (M = Ag, Au, Cu, Rh and Ru) clusters: A density functional theory study**

Fellah M. F. , ÖNAL I.

CATALYSIS TODAY, vol.171, pp.52-59, 2011 (Journal Indexed in SCI)

- **An ONIOM and DFT Study of Water and Ammonia Adsorption on Anatase TiO<sub>2</sub> (001) Cluster**

Erdogan R., ÖNAL I.

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, vol.111, pp.2149-2159, 2011 (Journal Indexed in SCI)

- **Epoxidation of Ethylene by Silver Oxide (Ag<sub>2</sub>O) Cluster: A Density Functional Theory Study**

Fellah M. F. , van Santen R. A. , ÖNAL I.

CATALYSIS LETTERS, vol.141, pp.762-771, 2011 (Journal Indexed in SCI)

- **A DFT Study of Direct Oxidation of Benzene to Phenol by N<sub>2</sub>O over [Fe( $\mu$ -O)Fe](2+) Complexes in ZSM-5 Zeolite**

Fellah M. F. , Pidko E. A. , van Santen R. A. , ÖNAL I.

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- **A density functional theory study of C-H bond activation of methane on a bridge site of M-O-M-ZSM-5 Clusters (M = Au, Ag, Fe and Cu)**  
Kurnaz E., Fellah M. F. , ÖNAL I.  
MICROPOROUS AND MESOPOROUS MATERIALS, vol.138, pp.68-74, 2011 (Journal Indexed in SCI)
- **Ethylene Epoxidation Catalyzed by Silver Oxide**  
Ozbek M. O. , ÖNAL I., van Santen R. A.  
CHEMCATCHEM, vol.3, pp.150-153, 2011 (Journal Indexed in SCI)
- **An ONIOM and DFT Study of Water Adsorption on Rutile TiO<sub>2</sub> (110) Cluster**  
Erdogan R., Fellah M. F. , ÖNAL I.  
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, vol.111, pp.174-181, 2011 (Journal Indexed in SCI)
- **Investigation of ruthenium-copper bimetallic catalysts for direct epoxidation of propylene: A DFT study**  
Kizilkaya A. C. , Senkan S., ÖNAL I.  
JOURNAL OF MOLECULAR CATALYSIS A-CHEMICAL, vol.330, pp.107-111, 2010 (Journal Indexed in SCI)
- **A Density Functional Theory Study of Direct Oxidation of Benzene to Phenol by N<sub>2</sub>O on a [FeO](1+)-ZSM-5 Cluster**  
Fellah M. F. , ÖNAL I., van Santen R. A.  
JOURNAL OF PHYSICAL CHEMISTRY C, vol.114, pp.12580-12589, 2010 (Journal Indexed in SCI)
- **A periodic DFT study of water and ammonia adsorption on anatase TiO<sub>2</sub> (001) slab**  
Erdogan R., Ozbek O., ÖNAL I.  
SURFACE SCIENCE, vol.604, pp.1029-1033, 2010 (Journal Indexed in SCI)
- **A density functional theory study of ethylene adsorption on Ni-10(111), Ni-13(100) and Ni-10(110) surface cluster models and Ni-13 nanocluster**  
Yilmazer N. D. , Fellah M. F. , ÖNAL I.  
APPLIED SURFACE SCIENCE, vol.256, pp.5088-5093, 2010 (Journal Indexed in SCI)
- **A Density Functional Study of 1, 1, 5-Tris(4-dimethylaminophenyl)-3-methyl-divinylene**  
Fellah M. F. , ÖNAL I.  
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, vol.110, pp.1041-1047, 2010 (Journal Indexed in SCI)
- **Direct gas-phase epoxidation of propylene to propylene oxide through radical reactions: A theoretical study**  
Kizilkaya A. C. , Fellah M. F. , ÖNAL I.  
CHEMICAL PHYSICS LETTERS, vol.487, pp.183-189, 2010 (Journal Indexed in SCI)
- **Direct Methane Oxidation to Methanol by N<sub>2</sub>O on Fe- and Co-ZSM-5 Clusters with and without Water: A Density Functional Theory Study**  
Fellah M. F. , ÖNAL I.  
JOURNAL OF PHYSICAL CHEMISTRY C, vol.114, pp.3042-3051, 2010 (Journal Indexed in SCI)
- **New Catalytic Materials for the Direct Epoxidation of Propylene by Oxygen: Application of High-Throughput Pulsed Laser Ablation**  
Kahn M., Seubsai A., ÖNAL I., Senkan S.  
TOPICS IN CATALYSIS, vol.53, pp.86-91, 2010 (Journal Indexed in SCI)
- **Propylene Epoxidation: High-Throughput Screening of Supported Metal Catalysts Combinatorially Prepared by Rapid Sol-Gel Method**  
ÖNAL I., Duzenli D., Seubsai A., Kahn M., ŞEKER E., Senkan S.  
TOPICS IN CATALYSIS, vol.53, pp.92-99, 2010 (Journal Indexed in SCI)
- **High Throughput Synthesis and Screening of New Catalytic Materials for the Direct Epoxidation of Propylene**  
Kahn M., Seubsai A., ÖNAL I., Senkan S.  
COMBINATORIAL CHEMISTRY & HIGH THROUGHPUT SCREENING, vol.13, pp.67-74, 2010 (Journal Indexed in SCI)
- **Oxidation of Benzene to Phenol by N<sub>2</sub>O on an Fe<sup>2+</sup>-ZSM-5 Cluster: A Density Functional Theory Study**  
Fellah M. F. , van Santen R. A. , ÖNAL I.  
JOURNAL OF PHYSICAL CHEMISTRY C, vol.113, pp.15307-15313, 2009 (Journal Indexed in SCI)
- **A density functional theory study of oxidation of benzene to phenol by N<sub>2</sub>O on Fe- and Co-ZSM-5**

## clusters

Fellah M. F. , ÖNAL I.

TURKISH JOURNAL OF CHEMISTRY, vol.33, pp.333-345, 2009 (Journal Indexed in SCI)

- **A Density Functional Study of Ni-2 and Ni-13 Nanoclusters**

ÖNAL I., Sayar A., Uzun A., ÖZKAR S.

JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, vol.6, pp.867-872, 2009 (Journal Indexed in SCI)

- **N2O decomposition on Fe- and Co-ZSM-5: A density functional study**

Fellah M. F. , ÖNAL I.

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- **Synthesis of ZSM-5 from modified clinoptilolite and its catalytic activity in alkylation of benzene to ethylbenzene**

KARTAL Ö. E. , ÖNAL I.

CHEMICAL ENGINEERING COMMUNICATIONS, vol.195, pp.1043-1057, 2008 (Journal Indexed in SCI)

- **Activation of light alkanes on pure and Fe and Al doped silica clusters: A density functional and ONIOM study**

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- **A quantum chemical study of nitric oxide reduction by ammonia (SCR reaction) on V2O5 catalyst surface**

Soyer S., Uzun A., Senkan S., Onal I.

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- **Adsorption of water and ammonia on TiO2-anatase cluster models**

Onal I., Soyer S., Senkan S.

SURFACE SCIENCE, vol.600, pp.2457-2469, 2006 (Journal Indexed in SCI)

## Refereed Congress / Symposium Publications in Proceedings

- **Comparison between experiment and theory for methanol oxidation by vanadium-enzyme mimics**

Wachs I. E. , Molinari J., Gerceker D., ÖNAL I.

244th National Fall Meeting of the American-Chemical-Society (ACS), Pennsylvania, United States Of America, 19 - 23 August 2012, vol.244

## Supported Projects

ÖNAL I., Project Supported by Higher Education Institutions, FEN BİLİMLERİ ENSTİTÜSÜ/LİSANSÜSTÜ TEZ PROJESİ, 2014 - 2015

ÖNAL I., Project Supported by Higher Education Institutions, FEN BİLİMLERİ ENSTİTÜSÜ/LİSANSÜSTÜ TEZ PROJESİ, 2014 - 2015

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ÖNAL I., YALÇIN Ö., Project Supported by Higher Education Institutions, AMONYUM BORHİDRÜRÜN ZEOLİTLER ÜZERİNDE YENİDEN HİDROJENASYONU, 2013 - 2013

ÖNAL I., CİVAN A., Project Supported by Higher Education Institutions, OTOMOBİL EGSOZUNDAKİ HİDROKARBON, KARBON MONOKSİT VE AZOT OKSİT BİLEŞİKLERİNİN ARITILMASI İÇİN ÜÇ YOLLU KATALİTİK KONVERTERLERİN GELİŞTİRİLMESİ, 2013 - 2013

ÖNAL I., TEZSEVİN İ., Project Supported by Higher Education Institutions, ÇEŞİTLİ METAL OKSİT YÜZEYLERDE

PROPİLEN EPOKSİDASYONUNUN KUANTUM MEKANİK ÇALIŞMASI, 2013 - 2013

ÖNAL I., GÜLBİTER M., Project Supported by Higher Education Institutions, KARBON NANOTÜPLERİN KUANTUM KİMYASAL METHODLAR KULLANILARAK KATALİTİK ÜRETİMİ, 2013 - 2013

ÖNAL I., YETİŞEMİYEN P., Project Supported by Higher Education Institutions, ÜÇ YOLLU OTOMOTİV

KATALİZÖRLERİNİN DENEYSEL VE TEORİK ARAŞTIRMASI, 2013 - 2013

ÖNAL I., Project Supported by Higher Education Institutions, Egsoz Gazındaki Hidrokarbon , Karbon Monoksit Ve Azot Oksit (no) Bileşiklerinin Üç Yollu Katalitik Konverter İle Artırılması, 2012 - 2012

ÖNAL I., Project Supported by Higher Education Institutions, Organik Tepkimelerin Katalizör Yüzeyleri Üzerinde Kuantum Kimyasal Hesaplar Yapan Yazılımlar Kullanılarak Ve Deneysel Olarak İncelenmesi., 2011 - 2011

ÖNAL I., Project Supported by Higher Education Institutions, Kimyasal Tepkimelerin Kuantum Kimyasal Hesaplar Yapan Yazılım Ve Yüksek Performanslı Bilgisayar Kullanarak İncelenmesi, 2009 - 2010

## Citations

Total Citations (WOS):858

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