

# Mostafa Youssef

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Department of Mechanical Engineering  
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## EDUCATION

### Massachusetts Institute of Technology, Cambridge, USA

Ph.D., Nuclear Science and Engineering, September 2013

M.S., Nuclear Science and Engineering, June 2010

### Alexandria University, Alexandria, Egypt

B.S., Nuclear and Radiation Engineering, June 2006

## RESEARCH INTERESTS

Thermodynamics– Defects – Density functional theory – Semiconductor physics – Materials interfaces – Diffusion – Charge transfer – Electric conductivity – Thermal conductivity – Water – Phase transitions

## PROFESSIONAL APPOINTMENT

1. The American University in Cairo, Department of Mechanical Engineering, New Cairo, Egypt. **Assistant Professor**, July 2017-Present.
2. Massachusetts Institute of Technology, Department of Materials Science and Engineering, Cambridge, USA. **Research Affiliate**, August 2016-Present.
3. Massachusetts Institute of Technology, Laboratory for Material Chemomechanics, Cambridge, USA. **Postdoctoral Associate**, February 2015-August 2016.
4. Massachusetts Institute of Technology, Laboratory for Electrochemical Interfaces, Cambridge, USA. **Postdoctoral Associate**, October 2013-August 2016.
5. Massachusetts Institute of Technology, Cambridge, USA. **Research Assistant**, September 2008-September 2013.
6. Alexandria University, Alexandria, Egypt. **Demonstrator**, September 2006- December 2007.

## TEACHING EXPERIENCE

1. The American University in Cairo, New Cairo, Egypt. **Instructor** for ENGR2122 Fundamentals of Fluid Mechanics, ENGR3202 Engineering Analysis and Computation I, ENGR3322 Fundamentals of Thermofluids, September 2017 – December 2017.
2. Massachusetts Institute of Technology, Cambridge, USA. **Guest Lecturer** in 22.70 Materials for Nuclear Applications, May 2011 and May 2014.
3. The National Institute of Standard and Technology, Gaithersburg, USA. **Guest Lecturer** in 21<sup>st</sup> NIST Computer Modeling Workshop, August 2010.
4. Alexandria University, Alexandria, Egypt. **Demonstrator** for, Thermodynamics, Modern Physics, Nuclear Physics, Nuclear Reactor Physics, Mathematical Physics, September 2006 – December 2007.

## MENTORING

1. Massachusetts Institute of Technology, Cambridge, USA. **Co-mentoring graduate students:**
  - Jessica G. Swallow (with Prof. Krystyn J. Van Vliet, September 2015-August 2016). Scope; studying the interplay between lattice defects and strain in doped  $\text{CeO}_2$ . The work is part of Jessica's PhD.
  - Minh Dinh (with Prof. Bilge Yildiz, September 2015-August 2016). Scope; training on methods of modern theory of polarization and application to vacancies in ferroelectric  $\text{ZrO}_2$ . The work is part of Minh's PhD.
  - Jing Yang (with Prof. Bilge Yildiz, September 2014-August 2016). Scope; training on density functional theory methods and concepts of defect chemistry, and application on interfacial phenomena at oxides hetero-interfaces. The work resulted in a peer-reviewed publication, two conference presentations, and is part of Jing's PhD.
  - Ming Yang (with Prof. Bilge Yildiz, October 2013-August 2015). Scope; training on density functional theory methods and concepts of defect chemistry, and application on doping and diffusion in  $\text{ZrO}_2$ . The work resulted in a peer-reviewed publication and M.S. thesis of Ming.
  - Uuganbayar Otgonbaatar (with Prof. Bilge Yildiz, September 2011-June 2013). Scope; training on density functional theory methods and concepts of defect chemistry, and application on doping  $\text{ZrO}_2$  with Nb. The work was concluded in a peer-reviewed and M.Eng. thesis of Uuganbayar.

## PEER-REVIEWED PUBLICATIONS

1. M. Youssef, K. J. Van Vliet, and B. Yildiz, "Polarizing oxygen vacancies in insulating metal oxides under high electric field" **submitted**.
2. M. Youssef, B. Yildiz, and K. J. Van Vliet, "Thermomechanical stabilization of electron small polarons in  $\text{SrTiO}_3$  assessed by the quasiharmonic approximation" **Physical Review B** 95, 161110(R) (2017).
3. J. Yang, M. Youssef, and Bilge Yildiz, "Predicting point defect equilibria across oxide hetero-interfaces: model system of  $\text{ZrO}_2/\text{Cr}_2\text{O}_3$ " **Physical Chemistry Chemical Physics** 19, 3869 (2017).
4. M. Youssef, Ming Yang, and B. Yildiz, "Doping in the valley of hydrogen solubility: A route to designing hydrogen resistant zirconium alloys" **Physical Review Applied** 5, 014008 (2016).
5. A. Aryanfar, J. Thomas, A. Van der Ven, D. Xu, M. Youssef, J. Yang, B. Yildiz, and J. Marian, "Integrated computational modeling of water side corrosion in zirconium metal clad under nominal LWR operating conditions" **JOM** 68, 2900 (2016).
6. U. Otgonbaatar, W. Ma, M. Youssef, and B. Yildiz, "Effect of niobium on the defect chemistry and oxidation kinetics of tetragonal  $\text{ZrO}_2$ " **The Journal of Physical Chemistry C** 118, 20122 (2014).
7. M. Youssef and B. Yildiz, "Predicting self-diffusion in metal oxides from first-principles: The case of oxygen in tetragonal  $\text{ZrO}_2$ " **Physical Review B** 89, 024105 (2014).
8. M. Youssef and B. Yildiz, "Hydrogen defects in tetragonal  $\text{ZrO}_2$  studied using density functional theory" **Physical Chemistry Chemical Physics** 16, 1354 (2014).
9. M. Youssef, R. J.-M. Pellenq, and B. Yildiz, "Docking  $^{90}\text{Sr}$  radionuclide in cement: An atomistic modeling study" **Physics and Chemistry of the Earth, Parts A/B/C** 70-71, 39 (2014).
10. M. Youssef and B. Yildiz, "Intrinsic point-defect equilibria in tetragonal  $\text{ZrO}_2$ : Density functional theory analysis with finite-temperature effects" **Physical Review B** 86, 144109 (2012).
11. M. Youssef, R. J.-M. Pellenq, and B. Yildiz, "Glassy nature of water in an ultraconfining disordered material: The case of calcium-silicate-hydrate" **Journal of the American Chemical Society** 133, 2499 (2011).

## CONFERENCE PRESENTATIONS

1. M. Youssef, R. J.-M. Pellenq, and B. Yildiz, “Chloride ion binding to the surface of calcium-silicate-hydrate” Materials Research Society Fall Meeting, Boston, USA, 2009 *Poster*.
2. M. Youssef and B. Yildiz, “Immobilization mechanisms of dissolved ionic species in cement matrix” Materials Research Society Spring Meeting, San Francisco, USA, 2010 *Oral*.
3. M. Youssef, R. J.-M. Pellenq, and B. Yildiz “Immobilization mechanisms of radioactive species in cement matrix: The case study of  $^{90}\text{Sr}$ ” The 3<sup>rd</sup> International Forum on Multidisciplinary Education and Research for Energy Science, Ishigaki-jima, Japan, 2010 *Oral*.
4. M. Youssef and B. Yildiz, “Effect of Li on zirconium alloy corrosion- Li insertion, and ion migration in  $\text{ZrO}_2$ ” Materials Research Society Fall Meeting, Boston, USA, 2011 *Oral*.
5. M. Youssef and B. Yildiz, “ $\text{ZrO}_2$  passive layer stability loss in the presence of hydrogen defects- Connections to pit initiation” Electrochemical Society 222<sup>nd</sup> Meeting, Honolulu USA, 2012 *Oral*.
6. M. Youssef and B. Yildiz, “Mechanical degradation of  $\text{ZrO}_2$  passive layer in the presence of hydrogen defects” Materials Research Society Fall Meeting, Boston, USA, 2012 *Poster*.
7. M. Youssef and B. Yildiz, “Mechanistic modeling of corrosion and hydrogen pickup: density functional theory analysis of oxygen diffusion and hydrogen defects in  $\text{ZrO}_2$ ” International Workshop on Structural Materials for Innovative Nuclear Systems, Idaho Falls, USA, 2013 *Poster*.
8. M. Youssef and B. Yildiz, “Designing hydrogen pickup resistant zirconium alloys starting from electrons” Materials Research Society Fall Meeting, Boston, USA, 2013 *Oral*.
9. M. Youssef and B. Yildiz, “The role of transition metal dopants in hydrogen pickup kinetics at the  $\text{ZrO}_2/\text{H}_2\text{O}$  interfaces: A density functional theory study”, TMS 143<sup>rd</sup> Meeting, San Diego, USA, 2014 *Oral*.
10. M. Youssef and B. Yildiz, “The volcano of hydrogen pickup in zirconium alloys explained by p-type doping of the passive oxide layer” Multiscale Materials Modeling meeting, Berkeley, USA, 2014 *Oral*.
11. M. Youssef and B. Yildiz, “Understanding pitting in the passive layer of carbon steel starting from first principles study of its point defects” Multiscale Materials Modeling meeting, Berkeley, USA, 2014 *Poster*.
12. M. Youssef and B. Yildiz, “Doping on the valley of hydrogen solubility: A route to design hydrogen resistant zirconium alloys” Materials Research Society Fall Meeting, Boston, USA, 2014 *Oral*.
13. M. Youssef and B. Yildiz, “Point defect equilibria and diffusion in siderite ( $\text{FeCO}_3$ ) passive film studied using density functional theory” Electrochemical Society 227<sup>th</sup> Meeting, Chicago USA, 2015 *Oral*.
14. M. Youssef, B. Yildiz, and K. J. Van Vliet, “Thermodynamics and electronic Structure of  $\text{SrTiO}_3$  ionic and electronic defects” Materials Research Society Fall Meeting, Boston, USA, 2015 *Oral*.
15. M. Youssef, M. Yang, B. Yildiz, “Doping on the valley of hydrogen solubility: A route to design hydrogen resistant zirconium alloys” TMS 145<sup>th</sup> Meeting, Nashville, USA, 2016 *Oral*.
16. M. Youssef, K. J. Van Vliet, and B. Yildiz, “Hydrostatic stress-temperature diagrams for electronic charge carriers in  $\text{SrTiO}_3$ ” Electrochemical Society 229<sup>th</sup> Meeting, San Diego USA, 2016 *Oral*.
17. M. Youssef, B. Yildiz, K. J. Van Vliet, “Thermodynamics and chemomechanics of electron polarons in  $\text{SrTiO}_3$ ” Materials Research Society Fall Meeting, Boston, USA, 2016 *Oral*.

## SYNERGISTIC ACITIVITIES

### 1. Awards

- Swan Top Student Prize, Alexandria University, Egypt, 2007.
- Egypt's Professional Engineers Syndicate Top Student Award, 2006.
- Egypt Award for Academic Distinction, Faculty of Engineering, Alexandria University, 2001-2006.

### 2. Invited Talks

- “Predicting charged defect equilibria using density functional theory” Talk in Professor Harry L. Tuller group at MIT, Cambridge, USA, 2014.

### 3. Conference Organization

- Session chair, Symposium: Electro-Chemo-Mechanics, Multiscale Materials Modeling meeting, Berkeley, USA, 2014.
- Session chair, Symposium: Computational Thermodynamics and Kinetics, TMS 145<sup>th</sup> Meeting, Nashville, USA, 2016.
- Session chair, Symposium: Mechano-Electro-Chemical Coupling in Energy Related Materials and Devices 2 , Electrochemical Society 229<sup>th</sup> Meeting, San Diego USA, 2016.

### 4. Journal Reviewer

- Journal of Electroceramics; Physical Chemistry Chemical Physics; Acta Materialia.

### 5. Computational Grants

- PI Proxy, “Density Functional Theory Study of Complex Oxides under Mechanical Stresses and Electric Fields”, 1,250,000 Service Units, Project m2309, DOE-NERSC, January 2017- January 2018.
- PI, “Density Functional Theory Study of Defect Thermodynamics and Kinetics in Compound Semiconductors”, 1,149,181 Service Units whose value is \$39,780,72, Project DMR140065, NSF-XSEDE, July 2015- December 2016.
- PI Proxy, “Density Functional Theory Study of Complex Oxides under Mechanical Stresses and Electric Fields”, 1,250,000 Service Units, Project m2309, DOE-NERSC, January 2016- January 2017.
- PI, “Density Functional Theory Study of The Thermodynamics and Kinetics of Pitting in Iron Passive Layer”, 557,473 Service Units whose value is \$19,299.48, Project DMR140065, NSF-XSEDE, July 2014-June 2015.