

# Fatih G. Sen

## Education

- 2007–2013 **Ph.D. Engineering Materials**, *University of Windsor*, Windsor, ON, Canada, *Dissertation: Atomistic simulations to micro-mechanisms of adhesion in automotive applications*.  
Supervisors: Prof. Dr. Ahmet T. Alpas and Dr. Yue Qi
- 2003–2006 **M.Sc. Metallurgical and Materials Engineering**, *Middle East Technical University*, Ankara, Turkey, *Thesis: Non-equilibrium molecular dynamics of electromigration in aluminum and its alloys*.  
Supervisor: Prof. Dr. M. Kadri Aydinol
- 1999–2003 **B.Sc. Metallurgical and Materials Engineering**, *Middle East Technical University*, Ankara, Turkey.

## Interests and Highlights

- **Atomistic modeling of materials (DFT and MD) and finite element analysis.**
- **Computational materials design and machine learning methods in materials science.**
- **Correlating materials theory and experimental observations.**
- **Materials for energy, electronics and transportation applications.**
- **Metallurgical failure analysis and tribology of metals, composites and coatings.**
- **Production and characterization of bulk and nano scale materials including thin films and nanoparticles for improved mechanical, chemical and electrochemical properties.**
- **Image and big data analysis in materials science.**

## Research Experience

- May 2014 – Present **Postdoctoral Researcher**, ARGONNE NATIONAL LABORATORY, Lemont, IL.
- Developed empirical force fields using single and multi-objective optimization methods for nanomaterials and investigated electronic structure of grain boundaries in CdTe solar cells using atomistic simulation methods.
- Developed a first principles based variable charge force field using genetic algorithms that can predict bulk, surface, nanostructure and catalytic properties of IrO<sub>2</sub>. *A journal article was published.*
  - Investigated single and multi-objective local and global optimization methods for empirical force field fitting. *A journal article is in preparation.*
  - Implemented image analysis methods to construct atomistic models of grain boundaries and dislocation cores in CdTe from STEM images.
  - Modeled different grain boundary and dislocation core structures in CdTe using empirical force fields and density functional theory (DFT) calculations in collaboration with experimental research groups. Revealed the effect of grain boundaries on solar cell performance of CdTe. *Three journal articles are in preparation.*
  - Computed the Raman spectra of various Li-N-O compounds using DFT methods and revealed the atomistic mechanisms that result in capacity enhancements in Li-S batteries in collaboration with experimental studies. *A journal article is in preparation.*

October 2007 **Research Assistant**, UNIVERSITY OF WINDSOR, Windsor, ON.

- April 2014 Investigated solutions for different industrial materials related problems by synergistically combining experimental and atomistic simulation methods.
- Investigated surface stability of hydrogen- and fluorine-terminated diamond surfaces by constructing a surface phase diagram using DFT calculations. Evaluated surface bonding and electronic structures in relation to adhesion and friction properties. *A journal article was published.*
  - Designed and performed tribological experiments and atomistic simulations based on DFT between aluminum and diamond-like carbon (DLC) coatings and synergistically combined the results to elucidate adhesion and friction mechanisms. *Three journal articles were published.*
  - Studied chemical bonding and electronic structure of Al/diamond interfaces using DFT. Determined the interfacial reactions occurred by the applied contact pressure.
  - Analyzed the effect of oxygen termination on diamond surfaces to the Al/diamond interface electronic and bonding structures using DFT. *A collaborative GM report was published.*
  - Studied the effect of oxygen atmosphere on the elastic and plastic deformation mechanisms of single crystal Al nanowires using reactive (ReaxFF) molecular dynamics (MD) methods. *A journal article was published.*
  - Determined suitable alloying elements that can anchor Pt nanoparticles on carbon surfaces for fuel cell applications using DFT calculations. Systematically incorporated 25 different elements at the Pt/graphene interface and depicted the anchoring ability in relation to their effect on the electronic and bonding structure. *A journal article was published.*
  - Synthesized Pt nanoparticles on carbon substrates using solution based impregnation method. PVD coated TiO<sub>x</sub> films on carbon surfaces, determined their effect on the production of sub-nanometre Pt particles and analyzed the electrochemical activity in fuel cells.
  - Modeled nanoindentation of thin films using finite element method (Computational contact mechanics course final project).

January 2005 **Research Assistant**, MIDDLE EAST TECHNICAL UNIVERSITY, Ankara, Turkey.

- October 2007 Mastered different atomistic simulation methods including DFT and MD and computationally designed materials solutions for electromigration and hydrogen storage problems.
- Developed a molecular dynamics program that incorporated pseudopotential based electromigration force calculation to simulate electromigration failure in Al alloys. *A journal article was published.*
  - Computed diffusion properties of selected substitutional elements in aluminum using MD simulations and evaluated defect energies to systematically design alloying elements that can retard electromigration failure in aluminum interconnects. *A journal article was published.*
  - Investigated thermodynamic stability of CaMg<sub>2</sub> hydrides using DFT calculations to evaluate the hydrogen storage capacities of CaMg<sub>2</sub> hydrides in relation to their electronic structure. *A conference proceeding was published.*
  - Performed DFT calculations to investigate the effect of substitutional elements on the formation enthalpy of FeTi hydrides and systematically designed alloying elements that can increase the hydrogen storage capacity of FeTi. *A conference proceeding was published.*

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## Awards, Scholarships and Honors

- 2013 Paper spotlighted in the "Highlights of 2012" in the Journal of Physics: Condensed Matter
- 2011 Nominee for the Best Poster Award in Materials Research Society Fall 2011 Meeting
- 2011 Ontario Graduate Scholarship (OGS), Summer 2011 – Winter 2012
- 2008 Materials Research Society Fall 2008 Meeting Outstanding Symposium Paper Award
- 2007 University of Windsor Doctoral Tuition Scholarship, Fall 2007 – Winter 2011

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## Academic and Administrative Experience

- July 2012 – **Research Project Coordinator**, UNIVERSITY OF WINDSOR, Windsor, ON.  
April 2014 Coordinated and organized research activities in the Tribology of Materials Research group.
- Coordinated and assisted research activities in a group of 20 researchers between Windsor and collaborating institutes.
  - Organized and led multiple projects while managing budget constraints.
  - Managed laboratory resources, maintained laboratory safety, installed and maintained laboratory equipment. Trained students for research and laboratory equipment usage.
  - Administered the group web site.
  - Assisted in writing technical reports and proposals.
- September 2011 – **Student Representative**, UNIVERSITY OF WINDSOR, Windsor, ON.  
August 2012 Represented the graduate students of the department in the departmental council and faculty coordinating council.
- January 2005 **Research Assistant**, MIDDLE EAST TECHNICAL UNIVERSITY, Ankara, Turkey.  
– October 2007 Worked in various departmental duties as a computer administrator, web site developer/administrator and SEM laboratory operator.

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## Teaching Experience

- January 2008 **Graduate Teaching Assistant**, UNIVERSITY OF WINDSOR, Windsor, ON.  
– August 2011 Assisted and provided guidance to undergraduate students on different engineering courses.
- **06-85-131 Computer-Aided Design** *Winter 2008* Assisted in laboratory work, marking, and tutoring in the course for teaching principles of engineering design for freshman students.
  - **06-92-459 Computer-Aided Engineering - CAE** *Summer 2008, 2009, 2010, 2011* Assisted in laboratory sessions and marking in the course for mechanical design and stress analysis with finite element modeling using CATIA V5.
  - **06-85-217 Mechanics Of Deformable Bodies I** *Fall 2008* Assisted in tutorials and marking in the course for static and strength analysis of engineering structures.
  - **06-92-222 Analysis of Mechanical Systems** *Winter 2010, 2011* Assisted in laboratory and marking in the course for numerical methods for engineering applications using MATLAB.
- January 2005 **Teaching Assistant**, MIDDLE EAST TECHNICAL UNIVERSITY, Ankara, Turkey.  
– October 2007 Assisted and provided guidance to graduate and undergraduate students.
- **METE222 Materials Science and Engineering** Assisted in tutorials and marking in teaching fundamentals of materials science,
  - **METE545 Atomistic Computer Modelling of Materials** Assisted in laboratory sessions and marking in the course for atomistic modeling of materials including MD and DFT methods.
  - **METE472 Corrosion and Oxidation of Metals** Assisted in marking in the course for fundamentals of corrosion.
  - **METE417 Computer Applications in Metallurgy** Assisted in marking in the course for computer programming for extractive metallurgy applications.

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## Internships

- July 2002 – **Summer Intern**, TUBITAK MARMARA RESEARCH CENTRE, Gebze, Turkey.  
August 2002 Conducted research on manufacturing industrial parts using investment casting method.
- July 2001 – **Summer Intern**, ERDEMIR, EREGLI IRON AND STEEL CO., Eregli, Turkey.  
August 2001 Assisted in the quality control processes in iron and steel production.

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## Computer skills

- Languages FORTRAN, C, VISUAL BASIC, HTML, L<sup>A</sup>T<sub>E</sub>X, SQL, MATLAB, PYTHON  
Programs MICROSOFT WINDOWS SERVER, LINUX/UNIX, MICROSOFT OFFICE, ADOBE PHOTOSHOP, HIGH PERFORMANCE/GRID COMPUTING

Scientific VASP, ABINIT, LAMMPS, REAXFF, GULP, MATERIALS STUDIO, R.I.N.G.S., ABAQUS, CATIA V5, ORIGIN PRO, SIGMAPLOT, MATHCAD, TECPLOT

## Materials Testing and Processing Skills

Microscopy SEM, TEM, FIB, Optical microscopy, Optical profilometry  
Spectroscopy XPS, Raman, EDS, FTIR, RBS, ERD  
Testing Pin-on-disk tribology, Scratch test, Nanoindentation, Calotest, Sessile-drop, Tribology in vacuum, Electrochemistry  
Production Thin films by PVD and solution based methods, Nanoparticles by impregnation method

## Languages

Turkish **Native**  
English **Fluent**  
German **Basic**

## Memberships

2006–Present Materials Research Society (MRS) Student Member  
2008–Present American Physical Society (APS) Student Member  
2009–Present Canadian Institute of Mining, Metallurgy and Petroleum Student Member  
2012–Present Materials Advantage (ACerS, AIST, ASM International, TMS) Student Member

## Interests

- Mountaineering  
- Table Tennis  
- Trekking  
- History and Literature

## Publications

### Refereed Journal Articles

- 2015 12. **F.G. Sen**, A. Kinaci, B. Narayanan, S.K. Gray, M.J. Davis, S.K.R.S. Sankaranarayanan, M.K.Y. Chan, "Towards accurate prediction of catalytic activity in IrO<sub>2</sub> nanoclusters via first principles-based variable charge force field", *Journal of Materials Chemistry A* 3 (2015) 18970.
- 2015 11. S. Bhowmick, **F.G. Sen**, A. Banerji, A.T. Alpas, "Friction and adhesion of fluorine containing hydrophobic hydrogenated diamond-like carbon (F-H-DLC) coating against magnesium alloy AZ91", *Surface and Coatings Technology* 267 (2015) 21.
- 2014 10. **F.G. Sen**, Y. Qi, A.C.T. Van Duin, A.T. Alpas, "Oxidation-assisted ductility in aluminum nanowires", *Nature Communications* 5 (2014) 3959.
- 2013 9. **F.G. Sen**, Y. Qi, A.C.T. Van Duin, A.T. Alpas, "Oxidation induced softening in Al nanowires", *Applied Physics Letters* 102 (2013) 051912.
- 2013 8. **F.G. Sen**, X. Meng-Burany, M. Lukitsch, Y. Qi, A.T. Alpas, "Low friction and environmentally stable diamond-like carbon (DLC) coatings incorporating Si and F sliding against aluminum", *Surface and Coatings Technology* 215 (2013) 340.
- 2013 7. **F.G. Sen**, Y. Qi, A.T. Alpas, "Tribology of fluorinated diamond-like carbon coatings: first principles calculations and sliding experiments", *Lubrication Science* 25 (2012) 111.

- 2012 6. **F.G. Sen**, Y. Qi, A.T. Alpas, "Anchoring Pt on graphene using metallic adatoms: A first principles investigation", *Journal of Physics Condensed Matter* 24 (2012) 225003. Featured as "IOP Select".
- 2011 5. **F.G. Sen**, Y. Qi, A.T. Alpas, "Material transfer mechanisms between aluminum and fluorinated carbon interfaces", *Acta Materialia* 59 (2011) 2601.
- 2010 4. M. Shafiei, A.R. Riahi, **F.G. Sen**, A.T. Alpas, "Improvement of platinum adhesion to carbon surfaces using PVD coatings", *Surface and Coatings Technology* 205 (2010) 306.
- 2009 3. **F.G. Sen**, Y. Qi, A.T. Alpas, "Surface stability and electronic structure of hydrogen and fluorine terminated diamond surfaces: a first principles investigation", *Journal of Materials Research* 24 (2009) 2461, Featured as "Outstanding Symposium Paper".
- 2008 2. **F.G. Sen**, M. K. Aydinol, "Atomistic simulation of self-diffusion in Al and Al Alloys under electromigration conditions", *Journal of Applied Physics* 104 (2008) 073510.
- 2006 1. **F.G. Sen**, M.K. Aydinol, "Non-Equilibrium Molecular Dynamics Simulation of Electromigration in Aluminum Based Metallic Interconnects", *Turkish Journal of Engineering and Environmental Sciences* 30 (2006) 387.

#### Articles in preparation

1. A. Kinaci, B. Narayanan, **F.G. Sen**, M.J. Davis, S.K. Gray, S.K.R.S. Sankaranarayanan, M.K.Y. Chan, "Evolutionary Algorithm Search for Global Minimum Structures of Au Nano-Clusters", *Submitted*.
2. B. Narayanan, A. Kinaci, **F.G. Sen**, M.J. Davis, S.K. Gray, M.K.Y. Chan, S.K.R.S. Sankaranarayanan, "Describing the diverse geometries of gold nanoclusters – a first-principles based bond order potential", *Submitted*.
3. **F.G. Sen**, B. Narayanan, A. Kinaci, M.J. Davis, S.K. Gray, S.K.R.S. Sankaranarayanan, M.K.Y. Chan, "A comparative study of optimization strategies for force field fitting", *In preparation*.
4. C. Sun, G. Lian, J. Wang, T. Paulauskas, **F.G. Sen**, C. Buurma, M.K.Y. Chan, R.F. Klie, M.J. Kim, "Multiple core configurations of Lomer dislocations at CdTe bicrystal interface", *In preparation*.
5. H.-L. Wu, A. Kinaci, **F.G. Sen**, M.K.Y. Chan, A.A. Gewirth, "Effects of Nitrate Additives on the Electrode-Electrolyte Interface – A Combined Surface-Enhanced Raman Spectroscopy-First Principles Study", *In preparation*.

#### Conference Proceedings and Presentations

- 2015 23. **F.G. Sen**, C. Buurma, T. Pauluaskas, C. Sun, M. Kim, S. Sivananthan, R.F. Klie, M.K.Y. Chan, "Thermodynamics, structural stability, and electronic structure of grain boundaries in CdTe using STEM and atomistic simulations", *THE U.S. Workshop on the physics and chemistry of II-VI materials*, Chicago, IL, September 5-8 (2015).
- 2015 22. **F.G. Sen**, C. Buurma, T. Pauluaskas, C. Sun, M. Kim, S. Sivananthan, R.F. Klie, M.K.Y. Chan, "Atomistic simulations of grain boundaries in CdTe", *42<sup>nd</sup> IEEE Photovoltaic Specialists Conference*, New Orleans, LA, June 14-19 (2015).
- 2015 21. C. Buurma, **F.G. Sen**, T. Pauluaskas, C. Sun, M. Kim, S. Sivananthan, R.F. Klie, M.K.Y. Chan, "Creation and Analysis of Atomic Structures for CdTe Bi-crystal Interfaces by the Grain Boundary Genie", *42<sup>nd</sup> IEEE Photovoltaic Specialists Conference*, New Orleans, LA, June 14-19, (2015).
- 2015 20. T. Pauluaskas, C. Buurma, C. Sun, M.K.Y. Chan, M. Kim, **F.G. Sen**, R.F. Klie, "A Fundamental Study of the Effects of Grain Boundaries on Performance of Poly-Crystalline Thin Film CdTe Solar Cells", *42<sup>nd</sup> IEEE Photovoltaic Specialists Conference*, New Orleans, LA, June 14-19, (2015).

- 2015 19. **F.G. Sen**, A. Kinaci, B. Narayanan, M.J. Davis, S.K. Gray, S.K.R.S. Sankaranarayanan, M.K.Y. Chan, "IrO<sub>2</sub> surface and nanostructure stability from first principles and variable charge force field calculations", *Electrochemical Society Meeting*, Chicago, IL, May 24-28 (2015).
- 2015 18. **F.G. Sen**, B. Narayanan, A. Kinaci, M.J. Davis, S.K. Gray, S.K.R.S. Sankaranarayanan, M.K.Y. Chan, "Development of a variable charge force-field to gain atomistic insights into IrO<sub>2</sub> surfaces and nanoclusters", *Materials Research Society Spring 2015 Meeting*, San Francisco, CA, April 6-10 (2015).
- 2015 17. C. Buurma, T. Paulauskas, **F.G. Sen**, C. Sun, M. Kim, R. Klie, M.K.Y. Chan, "0+2 - A first principles study of interactions among point defects and grain boundaries in CdTe", *Materials Research Society Spring 2015 Meeting*, San Francisco, CA, April 6-10 (2015).
- 2015 16. B. Narayanan, A. Kinaci, **F.G. Sen**, M.J. Davis, M.K.Y. Chan, S.K.R.S. Sankaranarayanan, S.K. Gray "Size-dependent dimensionality effects and structures in Au nanoclusters using a novel empirical force field", *Materials Research Society Spring 2015 Meeting*, San Francisco, CA, April 6-10 (2015).
- 2015 15. M.K.Y. Chan, A. Kinaci, B. Narayanan, **F.G. Sen**, S.K. Gray, M.J. Davis, S.K.R.S. Sankaranarayanan "Force field development from first principles for materials design", *American Physical Society March 2015 Meeting*, San Antonio, TX, March 2-6 (2015).
- 2015 14. **F.G. Sen**, B. Narayanan, A. Kinaci, M.J. Davis, S.K. Gray, S.K.R.S. Sankaranarayanan, M.K.Y. Chan, "Evolutionary algorithms for parameterization of force fields", *Opportunities in Materials Informatics Workshop*, Madison, WI, February 9-10 (2015).
- 2013 13. **F.G. Sen**, S. Bhowmick, A.T. Alpas, "Tribology for manufacturing auto components: Atomistic mechanisms and coatings", *Auto21 2013 Conference*, Toronto, ON, May 22-23 (2013).
- 2012 12. **F.G. Sen**, X. Meng-Burany, M. Lukitsch, Y. Qi, A.T. Alpas, "Friction and adhesion of Si and F incorporating diamond-like-carbon (DLC) coatings sliding against aluminum", *39th International Conference on Metallurgical Coatings and Thin Films (ICMCTF-2012)*, San Diego, CA, April 23-27 (2012).
- 2011 11. **F.G. Sen**, Y. Qi, A.C.T. van Duin, A.T. Alpas, "Deformation of Al nanowires in an oxygen environment" *Materials Research Society Fall 2011 Meeting*, Boston, MA, November 28-December 2 (2011).
- 2011 10. **F.G. Sen**, Y. Qi, A.T. Alpas, "Tribology of fluorinated diamond-like carbon coatings", *6th Symposium on Functional Coatings and Surface Engineering (FCSE-2011)*, Montreal, QC, June 5-8 (2011).
- 2011 9. **F.G. Sen**, Y. Qi, A.T. Alpas, "Anchoring platinum on graphene using metallic adatoms", *American Physical Society March 2011 Meeting*, Dallas, TX, March 21-25 (2011).
- 2010 8. **F.G. Sen**, Y. Qi, A.T. Alpas, "Tribology of fluorinated diamond-like carbon coatings: first principles calculations and sliding experiments", *First International Brazilian Conference on Tribology TriboBr-2010*, Rio de Janeiro, Brazil, November 24-26 (2010).
- 2009 7. **F.G. Sen**, Y. Qi, A.T. Alpas, "Improvement of the Pt/graphene interface adhesion by metallic adatoms for fuel cell applications", *Materials Research Society Fall 2009 Meeting*, Boston, MA, November 30-December 4 (2009).
- 2009 6. **F. G. Sen**, Y. Qi, A.T. Alpas, "Adhesion and Friction between Fluorinated Diamond-like Carbon Coatings and Aluminum", *EUROMAT 2009*, Glasgow, UK, September 7-10 (2009).
- 2008 5. **F.G. Sen**, Y. Qi, A.T. Alpas, "Surface stability and electronic structure of hydrogen and fluorine terminated diamond surfaces: a first principles investigation", *Materials Research Society Fall 2008 Meeting*, Boston, MA, December 1-5 (2008).

- 2007 4. **F.G. Sen**, A. Kinaci, M.K. Aydinol, "Effect of Alloying Elements on the Formation of FeTiH<sub>4</sub>: An Ab initio Study", *Proceedings X. International Conference Hydrogen Materials Science and Chemistry of Carbon Nanomaterials*, Crimea, Ukraine, September 22-28 (2007).
- 2006 3. **F.G. Sen**, M.K. Aydinol, "Molecular Dynamics of Electromigration in Aluminum and Its Alloys", *Proceedings 13th International Metallurgy-Materials Congress and Exhibition*, Istanbul, Turkey, November 9-12 (2006).
- 2005 2. **F.G. Sen**, M.K. Aydinol, "Investigation of Electromigration Forces in Metals", *Proceedings 12th International Metallurgy-Materials Congress and Exhibition*, Istanbul, Turkey, September 28-October 2 (2005).
- 2005 1. **F.G. Sen**, M.K. Aydinol, "First principles study of C14 type Laves phase CaMg<sub>2</sub> hydrides", *Proceedings International Hydrogen Energy Congress and Exhibition IHEC 2005*, Istanbul, Turkey, July 13-15 (2005).

#### Reports and Book Chapters

- 2012 6. **F.G. Sen**, X. Meng-Burany, M. Lukitsch, Y. Qi, A.T. Alpas, "A new diamond-like carbon coating with humidity independent low friction against aluminum alloys" *General Motors Collaborative Report*, (March, 2012).
- 2011 5. H. Guo, Y. Qi, **F. G. Sen**, A. Abou Gharam, M.J. Lukitsch, A.T. Alpas, "The effect of oxygen on adhesion, adhesive transfer and friction of carbon coatings" *General Motors Collaborative Report CL-11/202/CML*, (August, 2011).
- 2010 4. **F.G. Sen**, Y. Qi, A.T. Alpas "Anchoring Pt catalyst on graphene by metallic adatoms" *General Motors Collaborative Report*, (November, 2010).
- 2010 3. **F.G. Sen**, Y. Qi, A.T. Alpas, "Adhesion of aluminum to fluorinated diamond-like carbon coatings", *General Motors Collaborative Report*, (April, 2010).
- 2009 2. **F.G. Sen**, A. Kinaci, M.K. Aydinol, "Effect of Alloying Elements on the Formation of FeTiH<sub>4</sub>: an Ab Initio Study" in book ed. by B. Baranowski et al. "*Carbon Nanomaterials in Clean Energy Hydrogen Systems*", p573-578 Springer, Netherlands (2009).
- 2008 1. **F.G. Sen**, Y. Qi, A.T. Alpas, "Surface stability and electronic structure of hydrogen and fluorine terminated diamond surfaces: a first principles investigation", *General Motors Collaborative Report* (November 2008).