



# SEDIGHEH BIGDELI

## INTRESETS

Modelling, Computational Thermodynamics and Kinetics, Quantum Physics, Ab-initio calculations

## ACADEMIC EXPERIENCES

**2017-present** Chalmers University of Technology, Gothenburg, Sweden  
Department of Chemistry and Chemical Engineering, Environmental Inorganic Chemistry  
*Postdoctoral researcher, working on kinetic modelling of oxidation of metals*

**2013- 2017** Kungliga Tekniska Högskolan (KTH), Stockholm, Sweden  
Department of Materials Science and Engineering  
*Post Graduate Education at Computational Thermodynamics Group, Generic Calphad project, as a part of Hero-m*  
PhD Thesis: Developing the 3<sup>rd</sup> generation of Calphad databases: what can ab-initio contribute?

**2010 - 2012** Kungliga Tekniska Högskolan (KTH), Stockholm, Sweden  
Department of Materials Science and Engineering  
*MSc Degree in Materials Science and Engineering*  
Master Thesis: Comparison of methods for examination of inclusion composition in stainless steel

**2002 - 2007** Amirkabir University of Technology (AUT), Tehran, Iran  
Department of Materials Science and Engineering  
*BSc Degree in Extractive Metallurgy Engineering*  
Bachelor Thesis: Water Adsorption of Organic Phase in Solvent Extraction of Copper by LIX984N

## ADVANCED COURSES

### PhD Courses

Phase transformation of high performance materials, Assessment of Thermodynamic Properties, Writing Scientific Articles, Quantum Metallurgy, Seminar Course in Atomic-Scale Materials Science, Diffusion in Multicomponent solids, High Performance Materials for Demanding Applications, Introduction to Analytical Electronic Microscopy, Applied Programming and Computer Science.

### Learning DFT calculations methods at Max-Planck-Institut für Eisenforschung, Dusseldorf, Germany, September-October 2015

2 months visit to learn and apply the DFT codes, TU-TILD and UP-TILD methods, to calculate thermodynamic properties of pure Mn in finite temperature.

### The Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Germany, November 2014

One week visit to learn DFT theory and Quantum Espresso software as a tool for DFT calculations

### Summer School at INSTN - CEA Saclay, France, July-2013

One week summer school about "Fundamentals of Thermodynamic Modelling of Materials", including several lectures and computer labs about first principle calculations, molecule dynamics, computational thermodynamics and phase field modelling, in France.

## AWARDS AND HONORS

**2013:** Accepted for the Post Graduate study in Computational Thermodynamics group, as a part of Hero-m, at Royal Institute of Technology, Sweden between more than 300 candidates

**2002:** Ranked 1700<sup>th</sup> out of more than 450,000 applicants for Engineering and Mathematical Science, Iran's mandatory university entrance examination

**1995:** Selected in National Organization for Development of Exceptional Talents (NODET) through

an exam among 700,000 participants

## QUALIFICATIONS

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- Level II Certificate of Quality Control of Welding Inspection (CWI) by AWS (American Welding Society) – graded 84% - December 2008
- Level II Certificate of Examination in Ultrasonic Testing (UT) by ASNT (American Society of Non-Destructive Testing) – graded 81% - August 2008.

## TEACHING AND ORGANIZATIONS

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- Lab assistant in course “Thermodynamics of materials” for undergraduate students Lab assistant in course “Applied thermodynamics and kinetics” for master students.
- Organizer of “The 7th, 8th and 9th annual Hero-m workshop”, in Stockholm with almost 80 participants, May 2014, 2015 and 2016.
- Organizer of frequent unary workshops at KTH, Stockholm November 2015, April and November 2016.
- Representative of PhD students (PAD) at leading group of materials science and engineering department, elected by PhD students, June 2015- Aug. 2016.
- Vice president in the board of Hera-n, a gender equality network at Jernkontoret for engineers within the area of materials technology, May 2014-December 2016.

## WORK EXPERIENCE

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- May 2012-December 2012, Outokumpu AB. Avesta, Sweden  
*Master thesis in Research and Development Department*
- August 2009 - August 2010, MAPNA Boiler Engineering and Manufacturing Co. Tehran, Iran.  
*Expert in a control project on the characterization and supply of raw materials*
- October 2007 - August 2009, Razi Metallurgical Research Center (RMRC), Tehran, Iran  
*Materials researcher in failure analysis, corrosion and life assessment investigations*

## SKILLS

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### Computer Skills:

- Professional in working with Computational Thermodynamic software (Calphad).
- Professional in working with DFT software; VASP, Quantum Espresso and EMTO.
- Knowledgeable in programming with Python, PASCAL and Matlab.

### Specific Skills:

- Experienced in working with Scanning Electron Microscope (SEM) and Inca Feature (IF), Optical Emission Spectrometry with Pulse Discrimination Analysis (OES-PDA), Electrolytic Extraction (EE) and other metallurgical devices and techniques

### Languages:

- **Persian** - Native
- **English** - Fluent
- **Swedish** - Fluent
- **Arabic** - Basics

## PUBLICATIONS

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[2017] Sedigheh Bigdeli, Qing Chen, and Malin Selleby, “A new description for pure C; in developing the third generation of Calphad databases”, Submitted to Journal of Phase Equilibria and Diffusion, JPED-17-09-2018.

[2017] Sedigheh Bigdeli and Malin Selleby, “A thermodynamic assessment of the binary Fe-Mn for the third generation of Calphad databases”, Submitted to CALPHAD- 2017-119.

[2017] Saman Nimali Gunasekara, Huahai Mao, Sedigheh Bigdeli, Justin NingWei Chiu, and Viktoria Martin, "Thermodynamic Assessment of Binary Erythritol-Xylitol Phase Diagram for Phase Change Materials Design", submitted to the CALPHAD-2017-96.

[2017] Toshihiro Omori, Sedigheh Bigdeli and Huahai Mao, "A generalized approach obeying the third law of thermodynamics for the expression of lattice stability and compound energy: a case study of unary Aluminum", submitted to CALPHA\_2017\_171.

[2016] Zhou Li, Sedigheh Bigdeli, Huahai Mao, Malin Selleby, "Thermodynamic evaluation of pure cobalt for the third generation of thermodynamic databases", *Physica Status Solidi (B)*, vol. 254, no. 2, pp. 16002231, 2017.

[2016] Sedigheh Bigdeli, Hossein Ehteshami, Qing Chen, Huahai Mao, Pavel Korzhavyi, Malin Selleby, "New description of metastable hcp phase for unaries Fe and Mn: Coupling between first principles calculations and CALPHAD modeling", *Physica status solidi (b)*, Vol. 253, Issue 9 pp. 1830–1836, 2016.

[2015] Sedigheh Bigdeli, Huahai Mao and Malin Selleby, "On the third generation Calphad databases: an updated description of Mn", *Physica status solidi (b)*, Vol. 252, pp. 2199-2208, 2015.

[2009] Parviz Davami and Sedigheh Bigdeli, "Ethics in Engineering", Published as Book by Sazman Sanjesh Iran, January 2009.

[2009] Parviz Davami and Sedigheh Bigdeli, "Mapping the Future of World, Journal of Academy of Science of Iran", No.11, March 2009.

## PRESENTATIONS

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**Sedigheh Bigdeli**, "3<sup>rd</sup> generation of Calphad databases – ongoing work at KTH", seminar at Caltech University, Los Angeles, USA, Feb. 2017.

**Sedigheh Bigdeli**, Albert Glensk, Blazej Grabowski, Alexandra Khvan, Huahai Mao, Malin Selleby, "Developing the third generation of Calphad databases - modelling Al as a case study", oral presentation at TMS conference 2017, San Diego, USA, 26 Feb-4 Mar.

**Sedigheh Bigdeli**, Sascha Maisel, Dominique Korbmacher, Blazej Grabowski, Huahai Mao, Qing Chen and Malin Selleby, "Creating a new generation of Calphad databases: Challenges and achievements", oral presentation at the Calphad XLV Conference, 29<sup>th</sup> May-1<sup>st</sup> June 2016, Awaji Island, Japan.

**Sedigheh Bigdeli**, Hossein Ehtashami, Huahai Mao, Andreas Blomqvist, Qing Chen, Pavel Korzhavyi, Malin Selleby, "Towards third generation Calphad databases: coupling between First Principles and Calphad calculations for case studies of Mn and Fe-Mn", oral presentation at Calphad XLIV Conference, 31<sup>st</sup> May-5<sup>th</sup> June 2015, Loano, Italy.

**Sedigheh Bigdeli**, Huahai Mao and Malin Selleby, "On the third generation Calphad databases: updated description of Mn and Fe-Mn", poster at Calphad XLIII Conference, 1-6<sup>th</sup> June 2014, Changsha, China.

## PERSONAL INTERESTS AND ACTIVITIES

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Painting, sport, running, martial art, hiking, reading, philosophy.