Curriculum Vitae

Mal–Soon Lee

August 28, 2009

1 Personal Data

Name	Mal–Soon Lee
Work address	Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, U.S.A.
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2 Research Experience

2009 - present	Postdoctoral research fellow. Advanced Material Research Institute, College of Sciences, University of New Orleans, New Orleans, LA 70148, U.S.A.

2007 - 2009 Postdoctoral research fellow.
Condensed Matter and Statistical Physics sector,
The Abdus Salam ICTP,
Italy

3 Teaching Experience

2008 I taught Numerical method course to diploma students in ICTP, Italy.

4 Education

2003 - 2008 Ph. D. in Physics.
University of Pune,
India
Advisor: Prof. D. G. Kanhere
Thesis title: `First principle calculations for electronic structure, equilibrium geometry, and finite temperature properties of small clusters.`

2005 - 2006 STEP – Ph. D. program.
The Abdus Salam ICTP,
Italy
Advisor: Prof. Sandro Scandolo

1991 - 1995 M. Sc. in Physics.
University of Delhi,
India

1983 - 1987 B. Sc. in Science.
Pusan National University,
Republic of Korea

5 Area of Research

Computational physics, *ab initio* molecular dynamics simulations, *ab initio* electronic structure calculations, high pressure physics, Thermoelectric materials.

- Half-Heusler semiconductors for thermoelectric materials

- High-pressure physics: first-principles simulations of phase transitions in molecular systems, with applications to materials science, geophysics and planetary science.
- Phonon, infrared and Raman spectra of various systems such as clusters, bulk systems.
- Surface science: first-principles calculations of surface reconstructions.
- Geometric and electronic structure of small clusters using first–principle calculations.
- Thermodynamic properties of small clusters by Born–Oppenheimer molecular dynamics simulations.

6 Skill Highlight

- Extensive experience in large–scale scientific/numerical computing, simulation and modeling.
- Proficiency in Fortran (F90).
- Experience in parallel computing using MPI.
- Experience in developing and porting codes on a range of Unix and GNU Linux platforms, PCs, SGI Itanium.
- Experience with libraries and packages such as LAPACK, BLAS, numerical recipes. Compilation of various codes like VASP and Quantum–ESPRESSO in P4 machines and Linux clusters. Experience with shell–scripts, LaTex, and graphic softwares such as gnuplot, xmgr.
- I have worked extensively with the VASP and Quantum–ESPRESSO packages for carrying out calculations during my research. I have modified Quantum–ESPRESSO (CP code) for my own calculations.
- I have an experience of using tools like conjugate gradient minimization, simulated annealing, Born–Oppenheimer and Car–Parrinello molecular dynamics, and analyzes of thermodynamics data using multiple histogram technique. I have also developed a suit of codes and scripts for analyzing the data generated by PwScf and FPMD/CP code of Quantum– ESPRESSO package as well as by VASP.

7 Scientific Production

7.1 Articles Published in Journals

1. **Mal–Soon Lee**, Javier A. Montoya, and Sandro Scandolo, *Thermodynamic stability of layered structures in compressed CO_2*, Phys. Rev. B. **79**, 144102 (2009).

2. Jian Sun, Dennis D. Klug, Roman Martonák, Javier Antonio Montoya, **Mal–Soon Lee**, Sandro Scandolo, and Erio Tosatti, *High-pressure polymeric phases of carbon dioxide*, Proc. Natl. Acad. Sci. U.S.A. **106**, 6077 (2009).

3. **Mal–Soon Lee**, F. Baletto, D. G. Kanhere, and S. Scandolo, *Far-infrared absorption of small water clusters by first-principles molecular dynamics*, J. Chem. Phys. **128**, 214506 (2008).

4. Seyed Mohammad Ghazi, **Mal-Soon Lee**, and D. G. Kanhere, *The effects of electronic structure and charged state on thermodynamic properties: An ab initio molecular dynamics investigations on neutral and charged clusters of Na_{39}, Na_{40}, and Na_{41}*, J. Chem. Phys. **128**, 104701 (2008).

5. **Mal–Soon Lee**, *et al.*, *$Si_xC_{1-x}O_2$ alloys: a possible route to stabilize carbon–based silica–like solids?*, Solid St. Comm. **144**, 273 (2007).

6. U. F. T. Ndongmouo, **M.-S. Lee**, R. Rousseau, F. Baletto, and S. Scandolo, *Finite-Temperature Effects on the Stability and Infrared Spectra of $HCl(H_2O)_6$ Clusters*, J. Phys. Chem. A **111**, 12810 (2007).

7. Shahab Zorriasatein, **Mal–Soon Lee** and D. G. Kanhere, *Electronic structures, equilibrium geometries, and finite-temperature properties of Na_n (n=39-55) from first principles*, Phys. Rev. B **76**, 165414 (2007).

8. **Mal–Soon Lee**, D. G. Kanhere, *Effects of geometric and electronic structure on the finite temperature behavior of Na_{58}, Na_{57}, and Na_{55} clusters*, Phys. Rev. B **75**, 125427 (2007).

9. **Mal–Soon Lee**, S. Gowtham, Haiying He, Kah–Chun Lau, Lin Pan, and D. G. Kanhere, *Geometry, electronic properties, and thermodynamics of pure and Al–doped Li clusters*, Phys. Rev. B **74**, 245412 (2006).

10. **Mal–Soon Lee**, S. Chacko, D. G. Kanhere, *First principle investigation of finite temperature behavior in small sodium clusters*, J. Chem. Phys. **123**, 164310 (2005).

11. **Mal–Soon Lee**, Kavita Joshi, and D. G. Kanhere, *Ab initio density–functional study of the equilibrium geometries and the electronic properties of $Li_{10-n}Sn_n$ (n=0-10) clusters*, Phys. Rev. A **72**, 015201 (2005).

7.2 Articles submitted or under preparation

1. **Mal–Soon Lee** and Sandro Scandolo, *Water-methane mixed liquid at extreme conditions*, in preperation.

2. Fontana M. Mateus, **Mal–Soon Lee**, and Sandro Scandolo, *Phase transition of liquid CO_2 at high pressure*, in preperation.

7.3 On going project

1. Impurity effect on thermodynamic properties of Al/Ga clusters.

2. Adsorption of H_2S on the Au(111) surface.

3. The dynamic properties of Ar clathrate hydrate.

4. Electronic structure and transport properties of half-Heusler systems.

5. Geometric and electronic properties of ionic clusters and their melting characteristics.

8 Schools Attended

2008 *63^{rd} Scottish Universities Summer School in Physics on "High Pressure Physics"*, Sabhal Mòr Ostaig Gaelic College, Isle of Skye, UK.

2008 *Advanced School on Quantum Monte Carlo Methods in Physics and Chemistry*, International Centre for Theoretical Physics, Trieste, Italy.

2007 *Spring College on Water in Physics, Chemistry and Biology*, International Centre for Theoretical Physics, Trieste, Italy.

2007 *Advanced School in High Performance Computing Tools for e-Science - joint DEMOCRITOS/INFM-eLab/SISSA-ICTP activity*, International Centre for Theoretical Physics, Trieste, Italy. (I have attended this school as a tutor for the first week.)

2006 *Bangalore Summer School on "Electronic Structure Methods and their Applications" in conjunction with Conference on Computational Materials Theory*, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India. (I have attended this school as a tutor.)

2006 *Tools for Computational Physics*, The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy.

9 Presentation

2009 *14^{th} International Workshop on Computational Physics and Materials Science*, The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy.

2008 *CPMD 2008 (Conference on modeling and computation of structure and dynamics of condensed phase systems)*, The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy.

2008 *63^{rd} Scottish Universities Summer School in Physics on "High Pressure Physics"*, Sabhal Mòr Ostaig Gaelic College, Isle of Skye, UK.

2006 *Bangalore Summer School on "Electronic Structure Methods and their Applications" in conjunction with Conference on Computational Materials Theory*, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India.

2006 *3^{rd} National Conference on Nanoscience and Nanotechnology*, International School for Advanced Studies, Trieste, Italy.

2005 *11^{th} International Conference on the Applications of the Density Functional Theory in Chemistry and Physics*, Geneva, Switzerland.

2005, 2006, 2007 *Raman Memorial Conference*, University of Pune, Pune, India. (I was awarded for the best presentation on 2007.)

10 Complementary Data

10.1 Other Career

1987–2000 I was a science teacher in high school.

1999 I was awarded as a educator with a good standard of science education from state department of education (Gyeoungsangnam-do Office of Education).

10.2 Languages

English(fluent), Korean(fluent), Hindi(conversation only)

References

- Prof. S. D. Mahanti
  Department of Physics and Astronomy,
  Michigan State University,
  East Lansing, MI 48824,
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- Prof. Puru Jena
  Department of Physics,
  Virginia Commonwealth University,
  Richmond, VA 23284,
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- Prof. Sandro Scandolo
  the Abdus Salam ICTP,
  Strada Costiera 11,
  34014 Trieste,
  Italy.
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- Dr. Roger Rousseau
  Fundamental and Computational Sciences Directorate,
  Pacific Northwest National Laboratory,
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