

Curriculum Vitae

Nicolas Douguet, PhD
Assistant Professor

• CONTACT INFORMATION

Kennesaw State University
Department of Physics
830 Polytechnic Lane, Academic Building
Marietta, GA 30060
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• EDUCATION

- Nov 2010: PhD in Physics, double-degree: Université Paris-Sud, France & University of Central Florida (UCF), Orlando, FL, Thesis: “*Symmetry in the dissociative recombination of polyatomic ions and in ultra-cold few body collisions*”
- Sep 2006: Master I of Sciences, Fundamental Physics, Université Paris-Sud, France
- May 2005: Bachelor of Science, Fundamental Physics, Université Paris-Sud, France
- May 2003: Pass entrance exam to the Engineering Schools “*Ecole des Ponts ParisTech*” and “*Télécom ParisTech*”
- Sep 2000 – Jun 2003: Classe préparatoire aux grandes écoles (Scientific preparatory school), Lycée Pasteur, France.
- June 1999: Baccalaureate, Speciality Mathematics

• RESEARCH WORK

- Aug 2019 – Present: Assistant Professor, Kennesaw State University, Marietta, GA
- Jul 2017 – Jul 2019: Research Associate, University of Central Florida, Orlando, FL
- June 2015 – June 2017: Postdoctoral fellow, Drake University, Des Moines, IA
- Jan 2011 – May 2015: Postdoctoral fellow, University of California, Davis, CA
- Sep 2009 – Mar 2010: Visiting research assistant, Laboratoire Aimé Cotton (CNRS), Orsay, France
- Jan 2007 – Nov 2010: Graduate Research Assistant, University of Central Florida
- Apr 2006 – Jun 2006: Experimental research internship in *Low-energy electron diffraction on material surfaces*, Laboratoire de Physique des solides (CNRS), Orsay, France

• TEACHING EXPERIENCE

- Aug 2019 – Present: Assistant Professor, Kennesaw State University, Marietta, GA,
PHY 3500K: Computational Physics, Spring 2020 & Spring 2021;
PHY 2212: Principles of Physics II, Fall 2019 & Fall 2020;
PHY 2212L: Physics II Laboratory, Spring 2020, Fall 2020 & Spring 2021.
- Aug – Dec 2016: Lecturer (instructor of records), *FYS 030: First year seminar: Energy for future presidents*, Drake University, Des Moines, IA

- Jan – May 2016: Lecturer (instructor of records), *PHY 122: Electromagnetic Theory*, Drake University, Des Moines, IA
- Jan – May 2016: Guest Lecturer, *PHY 121: Theoretical Mechanics*, 8 hours, Drake University, Des Moines, IA
- Aug – Dec 2015: Lecturer (instructor of records), *PHY 059: Advanced Laboratory I*, Drake University, Des Moines, IA
- Aug – Dec 2015: Guest Lecturer, *PHY 181: Quantum Theory*, 10 hours, Drake University, Des Moines, IA
- Jan – April 2015: Lecturer (co-teaching), *EME 115: Introduction to Numerical Methods and Analysis*, University of California, Davis, CA
- Aug – Dec 2010: Guest Lecturer, *PHY 4604: Wave Mechanics I*, 3 hrs, University of Central Florida, Orlando, FL
- Aug 2008 – Jan 2009: Graduate teaching assistant, *PHY 2049C: Physics for Engineers and Scientists II*, University of Central Florida, Orlando, FL
- Jan – May 2009: Guest Lecturer, *PHZ 3113: Introduction to Theoretical Methods of Physics*, 8 hrs, University of Central Florida, Orlando, FL

• GRANTS AND ACADEMIC ACHIEVEMENT

- Nov 2019: PI on the NSF proposal; “*Attosecond and strong field Physics in correlated multielectron systems*” (\$139,576)
- Nov 2018: Co-PI on the XSEDE-090031 proposal; “*Benchmark Calculations for Electron and Photon Collisions with Complex Atoms and Ions*”
- Nov 2018: Collaboration researcher on the NSF proposal; “*Decomposition of Organic Pollutants Using Electron Beams: A Theoretical Investigation*”
- Nov 2018: Project Assistant on the NSF proposal; “*Attosecond photoemission dynamics: novel ab initio methods for atomic and molecular ex-situ spectroscopies*”
- May 2016: Collaboration researcher on the FERMI proposal 20144078; “*Attosecond pulse shaping using a seeded FEL*”
- Mar 2014: Nominated for *Excellence in Postdoctoral Research*
- Aug 2008: Ranked first at the candidacy exam, University of Central Florida
- Mar 2007: National physics students Honor society - UCF chapter

• STUDENT MENTORING

- Feb 2021– Present: Mentor one undergraduate student (KSU); Michael Dodson.
- Aug 2020– Present: Mentor one undergraduate student (KSU); Taylor Moon.
- Jan 2020– May 2020: Mentor one undergraduate student (KSU); Zachary Delk.
- Sep 2017– Aug 2018: Mentor two Physics undergraduate students (UCF); Bejan Ghomashi and Jeremy Ponsot, leading to one peer-reviewed scientific publication in *Phys. Rev A*, a manuscript in preparation, and two conference posters, [M01.00045](#) and [M01.00046](#).
- Sep 2016 – June 2017: Mentor one Chemistry undergraduate student (Drake University); Erin McBroom, leading to one conference poster [Q1.00147](#).

- Sep 2015 – June 2017: Mentor one Physics undergraduate student (Drake University); Joel Venzke, leading to one conference presentation at DUCURS and [three peer-reviewed scientific publications](#) (cf. publication list).
- Apr – Jul 2008: Mentor one internship student (UCF); Elie Assémat, leading to one peer-reviewed scientific publication [*Complete symmetry characterization in collisions involving four identical atoms.*](#)

• ACADEMIC PARTICIPATION

- Nov 2020: Member of the PhD thesis defense committee of Hainan Liu : “*Theoretical study of electron collisions with NO₂ and N₂O molecules for control and reduction of atmospheric pollution*”, Université Paris-Saclay
 - Nov 2020: Member of the PhD thesis defense committee of Xian Wu Jiang: “*Hydrocarbon molecules databases for waste treatment applications*”, Université Paris-Saclay
 - 2020-2021: Member of the College awards committee, Kennesaw State University.
 - 2020-2021: Member of the Curriculum committee, Kennesaw State University.
 - 2019 - 2022: Member of the local organizing committee of ATTO22 conference, University of Central Florida.
 - Oct 2018: Participant in physics demonstrations for the [*UCF Physics Career Exploration day 2018*](#).
 - Apr 2018: Member of the undergraduate thesis committee of Bejan Ghomashi “*Resonant anisotropic emission in RABBITT spectroscopy*”.
 - Spring 2017: Participant in the First Year Seminar monthly meetings, Drake University
 - Fall 2016 - Spring 2017: Participant in the [*Scholarship of Teaching & Learning \(SoTL\)*](#), Drake University
 - Fall 2016: High-school Outreach Program: Visit of High Schools in West Des Moines to promote careers in Physics and Engineering.
 - Spring 2016: Member of the organization of the [*Drake Physics Prize*](#).
 - Mar 2007: National physics students Honor society - UCF chapter.
- RESEARCH INTERESTS: Attosecond spectroscopy; Ultra-fast and Strong-field physics; Control and time-resolved electron dynamics in multi-electron systems; High harmonic generation; Charge migration and electronic coherence in biomolecules; Time-resolved x-ray scattering, Light-assisted electron scattering, Circular dichroism in chiral systems.

• PUBLICATIONS

50. A. De Silva, T. Moon, K.L. Romans, B.P. Acharya, S. Dubey, K. Foster, O. Russ, C. Rischbieter, [N. Douguet](#), K. Bartschat, D. Fischer, submitted to Phys. Rev. A (2021) [*Circular Dichroism in Atomic Resonance-Enhanced Few-Photon Ionization*](#)
49. H. Gharibnejad, [N. Douguet](#), B. I. Schneider, J. Olsen, and L. Argenti, submitted to Comput. Phys. Commun. **263** 107889 (2021) [*A multi-center quadrature scheme for the molecular continuum*](#)
48. J. Fuchs, [N. Douguet](#), S. Donsa, F. Martín, J. Burgdörfer, L. Argenti, L. Cattaneo, and U. Keller, Phys. Rev. Research **3** 013195 (2021) [*Towards the complete phase profiling of attosecond wave packets*](#)

47. D. Bharti, D. Atri-Schuller, G. Menning, K. R. Hamilton, R. Moshammer, T. Pfeifer, N. Douguet, K. Bartschat, and A. Harth, Phys. Rev. A **103** 022834 (2021) *Decomposition of the transition phase in multi-sideband RABBITT schemes*
46. A. De Silva, D. Atri-Schuller, S. Dubey, B.P. Acharya, K.L. Romans, K. Foster, O. Russ, K. Compton, C. Rischbieter, N. Douguet, K. Bartschat, and D. Fischer, Phys. Rev. Lett. **126** 023201 (2021) *Using circular dichroism to control energy transfer in multi-photon ionization*
45. S. Meister, A. Bondy, K. Schnorr, S. Augustin, H. Lindenblatt, F. Trost, X. Xie, M. Braune, R. Treusch, N. Douguet, T. Pfeifer, K. Bartschat, and R. Moshammer, Phys. Rev. A **102** 062809 (2020) *Photoelectron spectroscopy of laser-dressed atomic helium*
44. T. Pauly, A. Bondy, K. R. Hamilton, N. Douguet, X.-M. Tong, D. Chetty, and K. Bartschat, Phys. Rev. A **102** 013116 (2020) *Ellipticity Dependence of Excitation and Ionization of Argon Atoms by Short-Pulse Infrared Radiation*
43. D. Chetty, R. D. Glover, B. A. deHarak, X.-M. Tong, H. Xu, T. Pauly, N. Smith, K. R. Hamilton, K. Bartschat, J. P. Ziegel, N. Douguet, A. N. Luiten, P. S. Light, I. V. Litvinyuk, and R. T. Sang, Phys. Rev. A **101** 053402 (2020) *Observation of Dynamic Stark Resonances in Strong-Field Excitation*
42. N. Douguet, S. Fonseca dos Santos and T. N. Rescigno, Phys. Rev. A **101** 033411 (2020) *Inner-shell photodetachment of Cn^- ions*
41. J. Fuchs, N. Douguet, S. Donsa, F. Martín, J. Burgdörfer, L. Argenti, L. Cattaneo, and U. Keller, Optica **7** 154 (2020) *Time delays from one-photon transitions in the continuum*
40. E. V. Gryzlova, M. M. Popova, A. N. Grum-Grzhimailo, E. I. Staroselskaya, N. Douguet, and K. Bartschat, Phys. Rev. A **100** 063417 (2019) *Coherent control of the photoelectron angular distribution in ionization of neon by a circularly polarized bichromatic field in the resonance region*
39. Z. Mezei, K. Chakrabarti, M. Epee Epee, O. Motapon, Y. Chi, A. Mehdi, N. Douguet, S. Fonseca dos Santos, V. Kokouline, and I. Schneider, ACS Earth Space Chem **3** 2376 (2019) *Electron-induced excitation, recombination and dissociation of molecular ions initiating the formation of complex organic molecules*
38. S. Donsa, N. Douguet, J. Burgdörfer, I. Brezinová, and L. Argenti, Phys. Rev. Lett. **123**, 133203 (2019) *Circular holographic ionization-phase meter*
37. A. N. Grum-Grzhimailo, N. Douguet, M. Meyer, and K. Bartschat, Phys. Rev. A **100** 033404 (2019) *Two-color XUV+NIR multi-photon near-threshold ionization of the helium ion by circularly polarized light in the region of the 3p resonance*
36. U. Satya Sainadh, H. Xu, X. Wang, A.-T. Noor, W. C. Wallace, N. Douguet, A. W. Bray, I. Ivanov, K. Bartschat, A. Kheifets, R. T. Sang, and I. V. Litvinyuk, Nature **567** 75 (2019) *Attosecond angular streaking and tunnelling time in atomic hydrogen*
35. C. H. Yuen, N. Douguet, S. Fonseca dos Santos, A. E. Orel, and V. Kokouline, Phys. Rev. A **99** 032701 (2019) *Simplified model to treat the electron attachment of complex molecules: Application to H_2CN and the quest for CN^- formation mechanism*
34. B. Ghomashi, N. Douguet, and L. Argenti, Phys. Rev. A **99** 053407 (2019), *Resonant anisotropic emission in RABBITT spectroscopy*

33. A. Harth, N. Douguet, K. Bartschat, R. Moshammer, and T. Pfeifer, Phys. Rev. A **99** 0233410 (2019) *Extracting phase information of continuum-continuum dipole transitions*
32. N. Douguet and K. Bartschat, Phys. Rev. A **99** 023417 (2019) *Attoclock setup with negative ions: A possibility for experimental validation*,
31. N. Douguet, B. I. Schneider, and L. Argenti, Phys. Rev. A **98** 023403 (2018) *Application of the complex Kohn variational method to attosecond spectroscopy*
30. A. Chew, N. Douguet, C. Cariker, J. Li, E. Lindroth, X. Ren, Y. Yin, L. Argenti, W. T. Hill, III, and Z. Chang, Phys. Rev. A (R) **97** 031407 (2018) *Attosecond transient absorption spectrum of argon at the $L_{2,3}$ edge*
29. E. V. Gryzlova, A. N. Grum-Grzhimailo, E. I. Staroselskaya, N. Douguet, and K. Bartschat, Phys. Rev. A **97** 013420 (2018) *Quantum coherent control of the photo-electron angular distribution in bichromatic ionization of atomic neon*
28. N. Douguet and K. Bartschat, Phys. Rev. A **97** 013402 (2018) *Dynamics of Tunneling Ionization using Bohmian Mechanics*
27. L. Giannessi, E. Allaria, K. C. Prince, C. Callegari, G. Sansone, K. Ueda, T. Morishita, C. Nan Liu, A. N. Grum-Grzhimailo, E. V. Gryzlova, S.I. Strakhova, N. Douguet and K. Bartschat, Sci. Rep., **8** 7774 (2018) *Soft x-ray coherent control schemes*
26. N. Douguet, K. Bartschat, E. V. Gryzlova, E. I. Staroselskaya, and A. N. Grum-Grzhimailo, Europ. J. Phys. D, **71** 105 (2017) *Photoelectron angular distribution in two-pathway ionization of Neon with femtosecond pulse*
25. M. Ilchen, N. Douguet, T. Mazza, A. J Rafipoor, C. Callegari, P. Finetti, O. Plekan, K. C. Prince, A. Demidovich, C. Grazioli, L. Avaldi, P. Bolognesi, M. Coreno, M. Di Fraia, M. Devetta, Y. Ovcharenko, S. Dusterer, K. Ueda, K. Bartschat, A. N. Grum-Grzhimailo, A. V. Bozhevolnov, A. K. Kazansky, N. M. Kabachnik, and M. Meyer, Phys. Rev. Lett. **118** 013002 (2017) *Circular dichroism in two-color resonant multi-photon ionization of oriented He^+ ions*
24. N. Douguet, A. N. Grum-Grzhimailo, and K. Bartschat, Phys. Rev. A **95** 013407 (2017) *Above threshold ionization in Neon induced by combining optical and bichromatic XUV femtosecond pulses*
23. M. Khamesian, N. Douguet, S. Fonseca dos Santos, O. Dulieu, M. Raoult, and V. Kokououline, Europ. J. Phys. D **70** 240 (2016) *Study of radiative electron attachment and photodetachment processes for the $\text{C}_2\text{H}/\text{C}_2\text{H}^-$ and $\text{C}_4\text{H}/\text{C}_4\text{H}^-$ molecules*
22. M. Khamesian, N. Douguet, S. Fonseca dos Santos, O. Dulieu, M. Raoult, W. J. Brigg and V. Kokououline, Phys. Rev. Lett. **117** 123001 (2016) *Formation of CN , C_3N , and C_5N^- molecules by radiative electron attachment and their destruction by photodetachment*
21. N. Douguet, E. Assemat and V. Kokououline, Europ. J. Phys. D **70** 228 (2016) *Complete symmetry characterization in collisions involving four identical atoms*
20. N. Douguet, A. N. Grum-Grzhimailo, E. V. Gryzlova, E. I. Staroselskaya, J Venzke and K. Bartschat, Phys. Rev. A **93** 033402 (2016) *Photoelectron angular distribution in bichromatic atomic ionization induced by circularly polarized VUV femtosecond pulses*
19. K. C. Prince, E. Allaria, C. Callegari, R. Cucini, G. De Ninno, S. Di Mitri, B. Diviacco, E. Ferrari, P. Finetti, D. Gauthier, L. Giannessi, N. Mahne, G. Penco, O. Plekan,

- L. Raimondi, P. Rebernik, E. Roussel, C. Svetina, M. Trov, M. Zangrando, M. Negro, P. Carpeggiani, M. Reduzzi, G. Sansone, A. N. Grum-Grzhimailo, E.V. Gryzlova, S.I. Strakhova, K. Bartschat, N. Douguet, J. Venzke, D. Iablonskyi, Y. Kumagai, T. Takanashi, K. Ueda, A. Fischer, M. Coreno, F. Stienkemeier, E. Ovcharenko, T. Mazza, M. Meyer, Nat. Photon. **10** 176 (2016) *Coherent control with a short-wavelength Free Electron Laser*
18. N. Douguet, D. S Slaughter, H. Adaniya, A. Belkacem, A. E. Orel and T. N. Rescigno, Phys. Chem. Chem. Phys. **17**, 25621 (2015) *Signatures of bond formation and bond scission dynamics in dissociative electron attachment to methane*
17. A. N. Grum-Grzhimailo, E. V. Gryzlova, E. I. Staroselskaya, S. I. Strakhova, J. Venzke, J. Conf. Series, ICPEAC (2015) N. Douguet and K. Bartschat, *Photoelectron angular distribution in bichromatic atomic ionization*
16. N. Douguet, S. Fonseca dos Santos, M. Raoult, O. Dulieu, A. E. Orel and V. Kokouline, J. Chem. Phys. **142**, 234309 (2015) *Theoretical study of radiative electron attachment to CN, C₂H and C₄H radicals*
15. S. Fonseca dos Santos, N. Douguet, A. E. Orel and T. N. Rescigno, Phys. Rev. A **91**, 023408 (2015) *Ligand effects in carbon-K-shell photoionization*
14. N. Douguet, S. Fonseca dos Santos, V. Kokouline and A. E. Orel, EPJ Web of Conferences **84**, 07003 (2015) *Simplified model to describe the dissociative recombination of linear polyatomic ions of astrophysical interest*
13. N. Douguet, V. Kokouline and A. E. Orel, Phys. Rev. A **90**, 063410 (2014) *Photodetachment cross sections of the C_{2n}H⁻ (n=1-3) hydrocarbon chain anions*
12. S. Fonseca dos Santos, N. Douguet, V. Kokouline and A. E. Orel, J. Chem. Phys. **140**, 0164308 (2014) *Scattering matrix approach to the dissociative recombination of HCO⁺ and N₂H⁺*
11. N. Douguet, M. Raoult, S. Fonseca dos Santos, O. Dulieu, A. E. Orel and V. Kokouline, Phys. Rev. A **88**, 052710 (2013) *Theory of radiative electron attachment to molecules: Benchmark study of CN⁻ Article selected by Phys. Rev. A as Editor's Suggestion*
10. N. Douguet, T. N. Rescigno and A. E. Orel, Phys. Rev. A **88**, 013412 (2013) *Carbon K-shell molecular-frame photoelectron angular distributions in the photoisomerization of neutral ethylene*
9. N. Douguet, T. N. Rescigno and A. E. Orel, Phys. Rev. A **86**, 013425 (2012) *Time-resolved molecular frame photoelectron angular distribution: Snapshots of aceylene-vinylidene cationic isomerization*
8. T. N. Rescigno, N. Douguet and A. E. Orel, J. Phys. B : At., Mol. Opt. Phys. **45**, 194001 (2012) *Imaging molecular isomerization using molecular-frame photoelectron angular distribution*
7. N. Douguet, V. Kokouline and A. E. Orel, . Phys. B : At., Mol. Opt. Phys., Fast track Comm., **45**, 051001 (2012) *Breaking a tetrahedral molecular ion with electrons: Study of NH₄⁺ Article selected by J. Phys. B editorial board as Highlights of 2012, IOP select*
6. N. Douguet, A. E. Orel, C. H. Greene and V. Kokouline, Phys. Rev. Lett. **108**, 023202 (2012) *Dissociative recombination of highly symmetric polyatomic ions*

5. N. Douguet, A. Orel, I.Mikhailov, I. Schneider , C. H. Greene and V. Kokouline, J. Phys.: Conf. Series **300** 012015 (2011) *The role of the Jahn-Teller coupling in dissociative recombination of H_3O^+ and H_3^+*
4. V. Kokouline, N. Douguet and C. H. Greene, Chem. Phys. Lett. **507**, 1 (2011) *Breaking bonds with electrons: dissociative recombination of molecular ions*
3. N. Douguet, V. Kokouline, and C. H. Greene, Phys. Rev. A **80**, 062712 (2009) *Theory of dissociative recombination of a linear triatomic ion with permanent electric dipole moment: Study of HCO^+*
2. N. Douguet, V. Kokouline, and C. H. Greene, Phys. Rev. A **77**, 064703 (2008) *Theoretical rate of dissociative recombination of HCO^+ and DCO^+*
1. N. Douguet, J. Blandon, and V. Kokouline, J. Phys. B: At. Mol. Opt. Phys. **41**, 045202 (2008) *Correlation diagrams in collisions of three identical particles*

- INVITED TALKS

- *Multiphoton ionization schemes using bicircular laser pulses*, June 4, 2020, The Division of Atomic and Molecular Physics 2020, Portland, OR (Virtual)
- *Ab initio numerical methods for attosecond and strong-field physics*, Dec 11, 2019, A Science Gateway for Atomic and Molecular Physics, Gaithersburg, Maryland
- *Ultrafast Physics in atoms and molecules in weak and strong fields*, March 1, 2019, Kennesaw State University, Marietta, GA
- *Light-induced Coherent Control and Ultra-fast Dynamics*, May 15, 2017, Stockholm University, Stockholm, Sweden (Virtual)
- *Light-induced Coherent Control and Ultra-fast Dynamics*, Feb 14, 2017, Kansas State University, Manhattan, KS
- *Electron and photon impact induced processes in Molecules*, Jan 5, 2017, Laboratoire Ondes et Milieux complexes, Université du Havre, Le Havre, France
- *Multi-photon two-color ionization of atoms and ions by femtosecond pulses*, The International Conference on Many Particle Spectroscopy of Atoms, Aug 23-28, 2016, Moscow, Russia
- *Electron-impact induced chemistry and coherent control of quantum phenomena with lasers*, Nov 30 2015, Drake University, Des Moines, IA
- *Electron-impact induced chemistry in Plasmas, Astrophysics and Biophysics*, Apr 2 2015, Sacramento State University, Sacramento, CA
- *Radiative electron attachment to molecules of astrophysical interest*, July 9 2013, The 9th international conference on dissociative recombination, Paris, France
- *Time-resolved molecular-frame photoelectron angular distribution (MFPAD): Snapshots of acetylene and ethylene photoisomerization*, Dec 4 2012, Institute for theoretical atomic molecular and optical physics (Harvard), workshop on “The theory of electron-molecule collisions for astrophysics, biophysics and low temperature plasmas: opportunities and challenges”, Cambridge, MA.
- *Breaking a tetrahedral molecular ion with electrons: Study of NH_4^+* , Feb 9 2012, The Roy. Soc. Disc, Meeting: Physics Chemistry, and Astronomy of H_3^+ , London, UK

- OTHER CONFERENCE CONTRIBUTIONS: Presented research work as oral and poster presentations at more than 20 scientific conferences worldwide.
- REFEREE FOR: Nat. Phys., Nat. Comm., Phys. Rev. Lett., J. Chem. Phys., Euro. Phys. J. D, J. Phys. B: At. Mol. Phys., and Phys. Rev. A
- MEMBER OF: the American Physical Society (APS) and Institute Of Physics (IOP)
- SPOKEN LANGUAGES: French (mother tongue), English (proficient), Portuguese (proficient) and German (good)
- CODES DEVELOPED:
 - SAE-TDSE: A single-active electron time-dependent Schrödinger equation code for strong-field photoionization in atoms with (*i*) random light polarization, (*ii*) a non-uniform grid method, and (*iii*) t-SURFF implementation (flux method).
 - LOPT-CK: A lowest-order perturbative method based on the Complex Kohn variational method to describe molecular photoionization with electron correlation involving up to three photon exchange.
 - ATTOMESA: A non-perturbative time-dependent code for molecular photoionization based on the MESA quantum chemistry code (ongoing development)
- IT SKILLS:
 - Operational systems: OS X, Unix, and Windows
 - Programming languages: C, C++, JAVA and FORTRAN
 - Quantum Chemistry codes: MESA, MOLPRO, and COLUMBUS