C. DAS PEMMARAJU

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Research Experience

Since 10/2014 Project scientist within the Ultrafast X-ray Science Laboratory, Chemical Sciences Division
Lawrence Berkeley National Laboratory, Berkeley, CA
Supervisors: Dr. Oliver Gessner and Dr. David Prendergast
Project Title: "*Theoretical interpretation of ultrafast time-resolved core-level spectroscopies using first-principles approaches*"

2013-2014 Materials project scientist within the Materials Sciences Division
Lawrence Berkeley National Laboratory, Berkeley, CA
Supervisor: Dr. David Prendergast
Project Title: "*Electronic structure of photovoltaic and photocatalytic materials through first principles simulations of core-level spectroscopies*"

2012-2013 Postdoctoral research fellow within the Chemical Sciences Division
Lawrence Berkeley National Laboratory, Berkeley, CA
Supervisor: Dr. David Prendergast
Project Title: "*Developing first-principles theory and simulation of f-electron soft x-ray spectroscopy for clean energy materials*"

2008-2012 Postdoctoral research fellow in Computational Spintronics
Trinity College Dublin, Ireland
Supervisor: Prof. Stefano Sanvito
Project Title: *"Implementation of advanced density functional methods for electronic structure and quantum transport."*

Education

2003-2008 Ph.D. in theoretical physics
Trinity College Dublin, Ireland
Supervisor: Prof. Stefano Sanvito
Thesis: "*Implementation of self-interaction free density functional methods and applications to dilute magnetic semiconductors.*"

2001-2003 Master of Science in Physics
Indian Institute of Technology Madras, Chennai, India
Supervisor: Prof. M.S.R Rao.
Thesis: "*Fabrication and study of electrical transport properties of LSMO/I/LSMO (I = STO/LHCMO) Magnetic Tunnel Junctions*"

1998-2001 Bachelor of Science in Mathematics, Physics and Computer Science
Andhra University, Vishakapatnam, India

Research Areas

2013-2014 First-principles methods for interpreting time-resolved core-level spectroscopies in clean energy materials

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X-ray photoemission spectroscopy at molecule-metal interfaces
Materials for lithium-ion flow batteries

2012-2013 Dye sensitized solar cells: Materials and charge transfer processes
Core-level spectroscopy of photocatalytic materials (α-Fe_2O_3, photosystem-II)
Co-ordination complexes for rare-earth separation
f-electron molecular magnetism

2011-2012 Constrained DFT for energy level alignment at nanoscale interfaces
Low-dimensional materials (MoS_2)

2009-2011 Charge transport in DNA
Spin polarized transport in magnetic molecules

2004-2009 Dilute magnetic semiconductors (DMS)
d^0 magnetism
Beyond-LDA methods in density functional theory

Mentoring experience

2012-2014 **Lawrence Berkeley National Laboratory, Berkeley**
Research Mentor to graduate and undergraduate students at the Molecular Foundry, LBNL

Regiane Nascimento, graduate student from from Universidade Federal de Minas Gerais, Brazil. 2014-
G_0W_0 calculations of quasiparticle spectra in B and N doped Graphene

Alison Altman, graduate student at UC Berkeley, 2013-
Simulation of Al K-edge x-ray absorption spectroscopy in cyclopentadienyl-aluminium complexes

Duan Ran, undergraduate summer intern from Peking University, 2012
G_0W_0 calculations on N-donor Uranyl co-ordination complexes
- Presented a poster at the 2013 MRS Spring meeting in San Francisco
- Currently attending graduate school at Cornell University

2009-2011 **Trinity College Dublin, Ireland**
Research Mentor to graduate students in the Computational Spintronics group

Kapildeb Dolui, graduate student, 2010-2012
First principles studies of the electronic structure of low-dimensional dichalcogenide materials
- Published two research articles in ACS Nano and Physical Review
- Currently pursuing postdoctoral studies in Singapore

Ismaeel Abdolhosseini Sarsari, visiting graduate student, 2010-2011
GW quasiparticle calculations on Cobalt doped ZnO
- Published a research article in Physical Review
- Currently Assistant Professor of Physics, Isfahan university of technology, Iran

Eduard Cremades, visiting graduate student from Universitat de Barcelona, 2009-2011
Spin transport in Mn_6 single molecule magnets
- Published a research article in Nanoscale
- Currently a school teacher in Spain

Teaching Experience

2009-2011 **Computational Laboratory supervisor,** Trinity College Dublin, Ireland
- Presented course material to students in a classroom setting
- Answered student queries as they carried out programming assignments

2005-2007 **Laboratory teaching assistant**, Trinity College Dublin, Ireland
- Demonstrated in junior and senior freshman undergraduate physics labs.
- Graded undergraduate lab reports
- Graded undergraduate physics tutorials

High performance computing experience

- ✓ Nearly 10 years of experience in Fortran based scientific software development for physics simulations
- ✓ Experienced in C, C++ and Java programming
- ✓ Extensive background in parallel programming for both distributed and shared memory architectures with MPI and OpenMP
- ✓ Experienced in code development based on public domain scientific libraries such as BLAS, LAPACK, ARPACK, PETSc, SCALAPAK, BLACS, FFTW, GSL etc and vendor optimized libraries such as Intel-MKL, ACML etc
- ✓ Experienced in debugging, profiling, porting and optimizing scientific computing codes for different architectures (Intel Xeon, Intel multicore, Cray, IBM Blue Gene, SGI Altix etc) and compilers (Intel, PGI, GNU, Cray etc)
- ✓ Familiar with CUDA based GPGPU programming
- ✓ Experienced in writing proposals for compute time allocations at large supercomputing facilities such as the DOE's National Energy Research Scientific Computing Center (NERSC), Irish Center for High-End Computing (ICHEC) etc.
- ✓ Knowledgeable in a wide variety of scripting languages such as bash, perl, awk, sed as well as web technologies such as javascript, jquery, ajax and php

Programming and large-scale code development experience

2004-2005 Implemented the atomic orbital self-interaction correction (ASIC) method within the numerical orbital based electronic structure package SIESTA. This scalable method has been since widely used within the computational spintronics group (CSG) at Trinity College Dublin (TCD) for a wide variety of applications ranging from magnetism in correlated oxides to quantum transport across molecules, magnetic tunnel junctions and ferroelectric heterostructures

2005-2006 Improved the parallelism in the diagonalization routines of SIESTA by implementing mixed-mode parallelism over both orbitals and k-points, optimizing the 2D block-cyclic data distribution within SCALAPACK and adding additional SCALAPACK drivers for performing parallel Divide and Conquer diagonalization.

2007-2008 Implemented within the SIESTA framework, optimized effective potential (OEP) based exact-exchange (EXX) and Self Interaction correction (SIC) at the KLI level for applications to molecular systems.

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2008-2009 Implemented an efficient mesh refinement algorithm within the *ab initio* electron transport code SMEAGOL in order to perform accurate numerical integrations of the sharp features in the Greens function over the real axis which are encountered in systems that are weakly coupled to the electrodes.

2009-2010 Incorporated into the SIESTA code, algorithms due to J. D.Talman [Int. J. Quantum Chem. 93, 72 (2003)] to evaluate two electron repulsion integrals over the fully numerical atomic orbital basis set employed within SIESTA.

2010-2011 Implemented a variational generalization of the ASIC method now termed VPSIC into SIESTA and extended the method further to handle non-collinear spin systems.

2011-2012 Programmed within SIESTA the capability to perform constrained density functional theory (CDFT) calculations to be used in applications involving charge transfer phenomena.

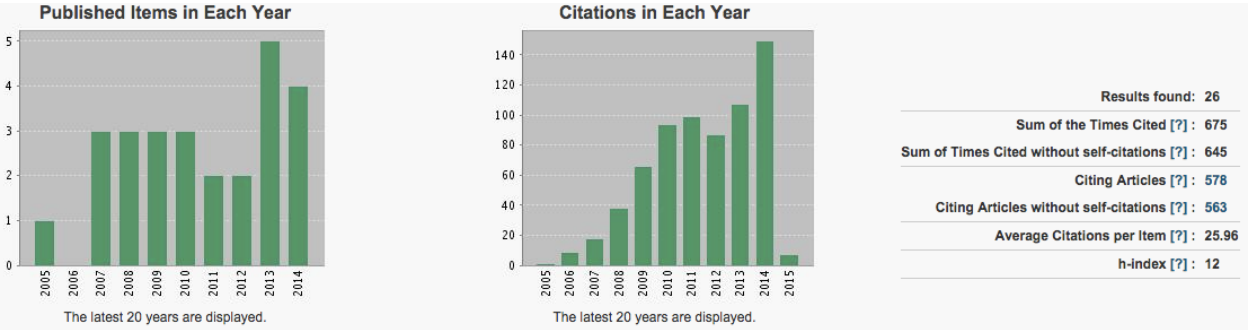
2012-2013 Extended the Quantum ESPRESSO based Shirley suite for X-ray spectroscopy [J. Chem. Phys. 140, 034107 (2014)] developed within the Prendergast group at LBNL, to spin-polarized systems and to take advantage of beyond semi-local exchange-correlation (XC) approximations. Interfaced the Shirley suite with the efficient G_0W_0 implementation within the GWL [http://gww.qe-forge.org] code.

2013-2014 Interfaced Quantum ESPRESSO with a versatile Poisson Solver [L. Genovese J. Chem. Phys, Vol. 127, p. 054704 (2007)] capable of handling hybrid boundary conditions in order to treat charged systems within the supercell approach in modeling X-ray photoemission spectroscopy. Implemented the handling of DFT+U into the pw2bgw interface between Quantum Espresso and BerkeleyGW.

Quantum mechanical simulation codes used: SIESTA, Quantum ESPRESSO, VASP, BerkeleyGW, Shirley, SMEAGOL, GAMESS, NWChem, QChem, Orca, OCTOPUS, ELK

Publication record:

Citation report: Total citations: 675, Current h-index: 12 (Thomson Reuters Web of Knowledge)



List of Publications

(1) *Attosecond band-gap dynamics in silicon.* Martin Schultze, Krupa Ramasesha, C.D. Pemmaraju, S.A. Sato, D. Whitmore, A. Gandman, James S. Prell, L. J. Borja, D. Prendergast, K. Yabana, Daniel M. Neumark, and Stephen R. Leone. *Science* 12 December 2014: **346** (6215), 1348-1352.

(2) *Bonding and Charge Transfer in Nitrogen-Donor Uranyl Complexes: Insights from NEXAFS Spectra.* C. D. Pemmaraju, Roy Copping, Shuao Wang, Markus Janousch, Simon. J. Teat, Tolek Tyliszcak, Andrew Canning, David K. Shuh, and David Prendergast, *Inorg. Chem.* **2014** 53 (21), 11415-11425

(3) *Atomic-Scale Perspective of Ultrafast Charge Transfer at a Dye–Semiconductor Interface.* Katrin R. Siefermann, Chaitanya D. Pemmaraju, Stefan Neppl, Andrey Shavorskiy, Amy A. Cordones, Josh Vura-Weis, Daniel S. Slaughter, Felix P. Sturm, Fabian Weise, Hendrik Bluhm, Matthew L. Strader, Hana Cho, Ming-Fu Lin, Camila Bacellar, Champak Khurmi, Jinghua Guo, Giacomo Coslovich, Joseph S. Robinson, Robert A. Kaindl, Robert W. Schoenlein, Ali Belkacem, Daniel M. Neumark, Stephen R. Leone, Dennis Nordlund, Hirohito Ogasawara, Oleg Krupin, Joshua J. Turner, William F. Schlotter, Michael R. Holmes, Marc Messerschmidt, Michael P. Minitti, Sheraz Gul, Jin Z. Zhang, Nils Huse, David Prendergast, and Oliver Gessner, *The Journal of Physical Chemistry Letters* **2014** *5* (15), 2753-2759

(4) *Towards equatorial planarity about uranyl; Synthesis and Structure of tridentate N-donor* $\{UO_2\}^{2+}$ *complexes.* Roy Copping, Byoungseon Jeon, **C. D. Pemmaraju**, Simon J. Teat, Markus Janousch, Tolek Tyliszczak, Andrew Canning, Niels Grønbech-Jensen, David Prendergast, and David K. Shuh, *Inorg. Chem.*, **2014**, *53* (5), pp 2506–2515

(5) *Constrained-DFT method for accurate energy-level alignment of metal/molecule interfaces,* A. M. Souza, I. Rungger, **C. D. Pemmaraju**, U. Schwingenschloegl and S. Sanvito, Phys. Rev. B **88,** 165112 (2013)

(6) *Possible doping strategies for* MoS_2 *monolayers: An ab initio study.* Kapildeb Dolui, Ivan Rungger, **C. D. Pemmaraju** and Stefano Sanvito, Phys. Rev. B **88,** 075420 (2013)

(7) *Spectroscopy of Donor-π-Acceptor Porphyrins for Dye-Sensitized Solar Cells,* Ioannis Zegkinoglou, Maria-Eleni Ragoussi, **C. D. Pemmaraju**, Phillip S. Johnson, David Pickup, J. Enrique Ortega, D. Prendergast, Gema de la Torre, F. J. Himpsel, *J. Phys. Chem. C*, **117**, 13357 (2013)

(8) *Many-body quasi-particle spectrum of Co doped ZnO: a GW perspective,* I. Abdolhosseini Sarsari, **C. D. Pemmaraju**, Hadi Salamati and S. Sanvito, Phys. Rev. B **87,** 245118 (2013)

(9) *Spin-Polarized Transport through single-molecule magnet* Mn_6 *Complexes*, Eduard Cremades , **C. D. Pemmaraju**, Stefano Sanvito and Eliseo Ruiz, Nanoscale **5,** 4751 (2013)

(10) *Electric Field Effects on Armchair* MoS_2 *Nanoribbons,* Kapildeb Douli, **Chaitanya Das Pemmaraju** and S. Sanvito, ACS *Nano,* **6** , 4823 (2012)

(11) *First-principles study of high-conductance DNA sequencing with carbon nanotube electrodes,* X. Chen, I. Rungger, **C. D. Pemmaraju**, U. Schwingenschlögl, and S. Sanvito Phys. Rev. B **85,** 115436 (2012)

(12) *Variational pseudo-self-interaction-corrected density functional approach to the ab initio description of correlated solids and molecules,* A. Filippetti, **C. D. Pemmaraju**, S. Sanvito, P. Delugas, D. Puggioni, V. Fiorentini, Phys. Rev. B **84,** 195127 (2011)

(13) *Exchange interactions and magnetic phases of transition metal oxides: Benchmarking advanced ab initio methods,* T. Archer, **C. D. Pemmaraju**, S. Sanvito, C. Franchini, J. He, A. Filippetti, P. Delugas, D. Puggioni, V. Fiorentini, R. Tiwari, and P. Majumdar, Phys. Rev. B **84,** 115114 (2011)

(14) *Ab initio study of electron transport in dry poly(G)-poly(C) A-DNA strands,* **C. D. Pemmaraju**, I. Rungger, X. Chen, A. R. Rocha, and S. Sanvito, Phys. Rev. B **82,** 125426 (2010)

(15) *Magnetic interaction of Co ions near the* $(10\bar{1}0)$ *ZnO surface,* T. Archer, **C. D. Pemmaraju** and S. Sanvito, New J. Phys. **12,** 083061 (2010)

(16) *Polaronic distortion and vacancy-induced magnetism in MgO,* A. Droghetti, **C. D. Pemmaraju**, and S. Sanvito, Phys. Rev. B **81,** 092403 (2010)

(17) *Ab initio calculation of the bias-dependent transport properties of Mn12 molecules,* **C. D. Pemmaraju**, I. Rungger, and S. Sanvito, Phys. Rev. B **80,** 104422 (2009)

(18) *Comment on "Theoretical Description of Carrier Mediated Magnetism in Cobalt Doped ZnO",* Stefano Sanvito and **Chaitanya Das Pemmaraju**, Phys. Rev. Lett. **102,** 159701 (2009)

(19) *Defect-Related Origin of the Ferromagnetism in ZnO:Co,* R. Hanafin, **C. D. Pemmaraju**, T. Archer, and S. Sanvito, Acta Physics Polonica A, **115,** 263 (2009)

(20) *Predicting d^0 magnetism: Self-interaction correction scheme,* A. Droghetti, **C. D. Pemmaraju**, and S. Sanvito, Phys. Rev. B **78,** 140404(R) (2008)

(21) *Impurity-ion pair induced high-temperature ferromagnetism in Co-doped ZnO,* **C. D. Pemmaraju**, R. Hanafin, T. Archer, H. B. Braun, and S. Sanvito, Phys. Rev. B **78,** 054428 (2008)

(22) *Polarizability of molecular chains: A self-interaction correction approach,* **C. D. Pemmaraju**, S. Sanvito, and K. Burke, Phys. Rev. B **77,** 121204(R) (2008)

(23) *Magnetic properties of ZrO_2-diluted magnetic semiconductors,* Thomas Archer, **Chaitanya Das Pemmaraju** and Stefano Sanvito, J. Mag. Mag. Mater, **316,** e188-e190 (2007)

(24) *Investigation of n-type donor defects in Co-doped ZnO,* **Chaitanya Das Pemmaraju**, Thomas Archer, Ruairi Hanafin and Stefano Sanvito, J. Mag. Mag. Mater, **316,** e185-e187 (2007)

(25) *Atomic-orbital-based approximate self-interaction correction scheme for molecules and solids,* **C. D. Pemmaraju**, T. Archer, D. Sánchez-Portal, and S. Sanvito, Phys. Rev. B **75,** 045101 (2007)

(26) *Ferromagnetism Driven by Intrinsic Point Defects in HfO_2,* **Chaitanya Das Pemmaraju** and S.Sanvito, Phys. Rev. Lett. **94,** 217205 (2005)

Manuscripts submitted or in preparation

(27) *Weakened Degeneracy Lifting Prompts Performance Enhancement in Hematite Homojunctions*, Ioannis Zegkinoglou[a], **C. D. Pemmaraju**, Xuefei Feng, Xiao Cheng, Jinghua Guo, F. J. Himpsel, Dunwei Wang, David Prendergast and Lionel Vayssieres [In preparation]

Invited Presentations

2014 **C. D. Pemmaraju** and David Prendergast, *Interpretation of ultrafast time-resolved core-level spectroscopies using static and time-dependent density functional theory approaches,* **Molecular Foundry User's Meeting 2014,** Berkeley, CA, August 2014

2010 **C. D. Pemmaraju**, A. Droghetti and S. Sanvito, *d^0 magnetism in self interaction corrected DFT.* **APS March meeting 2010**, Portland (USA), March 2010

2009 **C. D. Pemmaraju**, I. Rungger, and S. Sanvito. *Non-equilibrium electron transport in dry DNA,* ***QuantSim 09****, Warwick* (UK), August 2009

2009 **C. D. Pemmaraju**, I. Rungger, and S. Sanvito. *Non-equilibrium electron transport in dry DNA,* **IMRC 2009**, Cancun (Mexico), August 2009

2009 **C. D. Pemmaraju**, I. Rungger, and S. Sanvito. *Ab initio Simulations of the Transport Properties of Mn_{12} molecular magnets.* **2009 MRS Spring Meeting**, San Francisco (USA), April 2009