Anuj Goyal

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Research Interests

- Multi-scale computational (*ab initio* electronic structure, atomistic force-field, and Monte-Carlo) approaches for quantitative predictions of materials properties
- Develop knowledge on how defects (structure, chemistry, physics, thermodynamics, and kinetics) can help us tune or change material's intrinsic behavior for better functionality
- Machine learning techniques to solve long-existing as well as inverse design problems
- Complex metallic alloys for structural applications; Stable and metastable oxides, nitrides, chalcogenides, for electronics, computing, and clean energy applications

Education

Ph.D., Materials Science and Engineering 2011–2015
University of Florida, Gainesville, FL
Advisor: Prof. Simon R. Phillpot

M.S., Materials Science and Engineering 2010–2012
University of Florida, Gainesville, FL

B.Tech. & M.Tech., Metallurgical and Materials Engineering 2005–2010
IIT Madras, Chennai, India

Professional Appointments

Dec 2022	**Assistant Professor**, MSME Department, IIT Hyderabad, India
2019–2022	**Research Scientist II**, National Renewable Energy Laboratory, USA
2016–2019	**Postdoctoral Fellow**, Colorado School of Mines, USA
2015–2016	**Postdoctoral Associate**, University of Florida, USA

Sponsored Projects

1. **As PI:**
   Title: Harnessing charged-defect electronic entropy of water-splitting oxides for high H_2 yield
   Sponsoring Agency: SERB Start-up Research Grant (SRG)
   Period: Feb. 2024 - Jan. 2025
2. **As PI:**
   Title: Developing a computational approach to accelerate point-defects characterization in materials

Sponsoring Agency: IITH Seed Grant
Period: Aug. 2023–Jul. 2025

Publications

Google Scholar: https://scholar.google.com/citations?user=gA3HkFIAAAAJ

1. T. C. Douglas, M. J Dzara, A. JE Rowberg, K. A King, M. Syrigou, N. A Strange, R. T Bell, **Anuj Goyal**, Pin-W. Guan, R. B Wexler, J. B Varley, T. Ogitsu, S. Lany, A. H McDaniel, S. R Bishop, M. D Witman,"Large-scale experimental validation of thermochemical water-splitting oxides discovered by defect graph neural networks.", **Materials Horizons**, **2025**. DOI:10.1039/D5MH01566A.

2. Regier, C.E., O'Donnell, S., **Anuj Goyal**, Dzara, M.J., Park, J.E., Bell, R.T., Kramer, M.J., Paddison, J.A., Shulda, S., Ginley, D.S. and Yahne, D.R., "Interlayer Ions Control Spin Canting in Low-Dimensional Manganese Trimers in 12R-$Ba_4MMn_3O_12$ (M = Ce, Pr) Layered Perovskites", Inorganic Chemistry 63 (51), 24176-24186 **2024**. DOI:10.1021/acs.inorgchem.4c03915.

3. **Anuj Goyal**, Michael D. Sanders, Ryan P. O'Hayre, and Stephan Lany, "Predicting thermochemical equilibria with interacting defects: $Sr_{1-x}Ce_xMnO_{3-\delta}$ alloys for water splitting", **Physical Review X Energy** 3, 013008 **2024**. DOI: 10.1103/PRXEnergy.3.013008.

4. Ximeng Wang, **Anuj Goyal**, Peng Zhou, Elizabeth Gager, Dylan McCord, Juan C. Nino, Jonathan Scheffe, Stephan Lany, and Simon R. Phillpot, "$LaMnO_3$ dopants for efficient thermochemical water splitting identified by density functional theory calculations", **Journal of Physical Chemistry C** 127, 49, 23988 **2023**. DOI:10.1021/acs.jpcc.3c06835.

5. Matthew Witman*, **Anuj Goyal***, T. Ogitsu, A. H. McDaniel, and Stephan Lany, "Defect graph neural networks for materials discovery in high-temperature clean-energy applications", **Nature Computational Science** 3, 675-686 **2023**. DOI:10.1038/s43588-023-00495-2. (*authors contributed equally.)

6. S. Roychoudhury, S. Shulda, **Anuj Goyal**, R. Bell, S. Sainio, N. Strange, J. E. Park, E. N. Coker, S. Lany, D. Ginley, David Prendergast, "Investigating the Electronic Structure of Prospective Water-splitting Oxide $BaCe_{0.25}Mn_{0.75}O_{3-\delta}$ Before and After Thermal Reduction", **Chemistry of Materials** 35 (5), 1935-1947 **2023**.DOI: 10.1021/acs.chemmater.2c03139.

7. N. A. Strange, J. Park, **Anuj Goyal**, R. T. Bell, J. Trindell, J. D. Sugar, K. Stone, E. N. Coker, S. Lany, S. Shulda, and D. S. Ginley, "Formation of 6H-$Ba_3Ce_{0.75}Mn_{2.25}O_9$ during thermochemical reduction of 12R-$Ba_4CeMn_3O_{12}$:Identification of a polytype in the Ba(Ce,Mn)O_3 family", **Inorganic Chemistry** 61, 16, 6128-6137 **2022**. DOI:10.1021/acs.inorgchem.2c00282.

8. **Anuj Goyal**, Andriy Zakutayev, Vladan Stevanović and Stephan Lany, "Computational Fermi level engineering and doping-type conversion of Mg:Ga_2O_3 via three-step synthesis processing", **Journal of Applied Physics** 129, 245704 **2021**. DOI: 10.1063/5.0051788.

9. S. Sun, A. Tiihonen, F. Oviedo, Z. Liu, J. Thapa, N. T. P. Hartono, **Anuj Goyal**, C. Batali, A. Encinas, J. Yoo, R. Li, Z. Ren, M. Bawendi, V. Stevanović, J. Fisher and T. Buonassisi,

"A physical data fusion approach to optimize compositional stability of halide perovskites", **Matter** 4, 1-18, April 7, **2021**. DOI: 10.1016/j.matt.2021.01.008.

10. **Anuj Goyal**, Y. Li, A. Chernatynskiy, J. S. Jayashankar, M. C. Kautzky, S. B. Sinnott and S. R. Phillpot, "The influence of alloying on the stacking fault energy of gold from density-functional theory calculations", **Computational Materials Science** 188, 110236 **2020**. DOI: 10.1016/j.commatsci.2020.110236.

11. **Anuj Goyal**, P. Gorai, S. Anand, E. S. Toberer, G. J. Snyder and V. Stevanović, "On the dopability of semiconductors and governing material properties", **Chemistry of Materials** 32, 11, 4467-4480 **2020**. DOI:10.1021/acs.chemmater.9b05126.

12. P. Gorai, **Anuj Goyal**, E. S. Toberer and V. Stevanović, "A simple chemical guide for finding novel n-type dopable Zintl pnictide thermoelectric materials", **Journal of Materials Chemistry A** 7, 19385-19395 **2019**. DOI: 10.1039/C9TA03786A.

13. **Anuj Goyal**, K. Mathew, R. G. Hennig, A. Chernatynskiy, C. R. Stanek, S. T. Murphy, D. A. Andersson, S. R. Phillpot and B. P. Uberuaga, "The conundrum of relaxation volumes in first-principles calculations of charge defects in UO_2", **Applied Sciences** 9 (24), 5276 **2019**. DOI: 10.3990/app9245276.

14. J. Male, M. T. Agne, **Anuj Goyal**, S. Anand, I. T. Witting, V. Stevanović and G. J. Snyder, "The importance of phase equilibrium for doping efficiency: iodine doped PbTe", **Materials Horizons** 6 (7), 1444-1453 **2019**. DOI: 10.1039/C9MH00294D.

15. L. T. Schelhas, Z. Li, J. A, Christians, **Anuj Goyal**, P. Kairys, S. P. Harvey, D. H. Kim, K. H Stone, J. M. Luther, K. Zhu, V. Stevanović and J. J. Berry, "Insights into operational stability and processing of halide perovskite active layers", **Energy & Environmental Science** 12 (4), 1341-1348 **2019**. DOI: 10.1039/C8EE03051K.

16. **Anuj Goyal**, and V. Stevanović, "Metastable rocksalt ZnO is *p*-type dopable", **Physical Review Materials** 2, 084603 **2018**. DOI:10.1103/PhysRevMaterials.2.084603.

17. **Anuj Goyal**, S. McKechnie, D. Pashov, W. Tumas, M. van Schilfgaarde and V. Stevanović, "Origin of Pronounced Nonlinear Band Gap Behavior in Lead-Tin Hybrid Perovskite Alloys", **Chemistry of Materials** 30, 11, 3920-3928 **2018**. DOI:10.1021/acs.chemmater.8b01695.

18. **Anuj Goyal**, P. Gorai, E. S. Toberer and V. Stevanović, "First-principles calculation of intrinsic defect chemistry and self-doping in PbTe", **npj Computational Materials** 3, 42 **2017**. DOI: 10.1038/s41524-017-0047-6.

19. **Anuj Goyal**, P. Gorai, H. Peng, S. Lany, and V. Stevanović, "A computational framework for automation of point defect calculations", **Computational Materials Science** 130, 1-9 **2017**. DOI: 10.1016/j.commatsci.2016.12.040. **Editor's Choice**.

20. S. A. Miller, P. Gorai, B. R. Ortiz, **Anuj Goyal**, D. Gao, S. A. Barnett, T. O. Mason, G. J. Snyder, Q. Lv, V. Stevanović and E. S. Toberer, "Capturing anharmonicity in a lattice thermal conductivity model for high-throughput predictions", **Chemistry of Materials** 29, 6, 2494-2501 **2017**. DOI: 10.1021/acs.chemmater.6b04179.

21. Y. Li, **Anuj Goyal**, A. Chernatynskiy, J. S. Jayashankar, M. C. Kautzky, S. B. Sinnott and S. R. Phillpot, "Nanoindentation of gold and gold alloys by molecular dynamics simulations", **Materials Science and Engineering:A** 651, 346-357 **2016**. DOI: 10.1016/j.msea.2015.10.081.

22. **Anuj Goyal**, S. R. Phillpot, G. Subramanian, D. A. Andersson, C. R. Stanek and B. P. Uberuaga, "Impact of homogeneous strain on uranium vacancy diffusion in uranium dioxide", **Physical Review B** 91, 094103 **2015**. DOI: 10.1103/PhysRevB.91.094103.

23. K. Choudhary, T. Liang, A. Chernatynskiy, Z. Lu, **Anuj Goyal**, S. R. Phillpot and S. B. Sinnott, "Charge optimized many-body potential for aluminium", **Journal of Physics: Condensed Matter** 27, 015003 **2015**. DOI: 10.1088/0953-8984/27/1/015003.

24. **Anuj Goyal**, T. Rudzik, B. Deng, M. Hong, A. Chernatynskiy, S. B. Sinnott and Simon R. Phillpot, "Segregation of ruthenium to edge dislocations in uranium dioxide", **Journal of Nuclear Materials** 441, 96-102 **2013**. DOI: 10.1016/j.jnucmat.2013.05.031.

Honors and Awards

2021 **Key Contributor Award**, Materials Physics Group, MCCS Directorate, NREL, USA

2017 **Research work highlighted** at the Center for Next Generation of Materials Design, NREL, USA

2015 **Best Poster Presentation Award**, The Minerals, Metals and Materials Society (TMS), Orlando, USA

2014 **Outstanding International Graduate Student Award**, University of Florida, USA

2014 Awarded **Membership, Tau Beta Pi**, Engineering Honor Society

Teaching Experience

- Electronic Structure & Atomistic Modelling of Materials
- Computational Methods in Materials Science
- Fundamentals of Scientific Computing

Selected Invited Talks and Workshops

- "Predicting thermochemical equilibria with interacting defects in transition metal alloys for water splitting", **Gordon Research Conference on Defects in Semiconductors**, Newry, Maine, USA, August 6, **2024**
- "First Principles Modeling of Materials", **Workshop on Multiscale Modeling of AI/ML for Advanced Materials and Manufacturing Applications**, IIT Hyderabad, Telangana, India, July 25, **2024**
- "Computational Modeling of Point Defects in Semiconductors Using Density Functional Theory", **Workshop on Semiconductor Materials and Devices 2023**, IIT Hyderabad, Telangana, India, September 30, **2023**
- "Computational Approaches to Point Defects Modeling in Semiconductors", **Indian Institute of Science (IISc) Bangalore**, Karnataka, India, April 7, **2022**
- "Thermodynamic modeling of point defects", **North American Solid State Chemistry Conference (NASSCC)**, Golden, CO, USA, July 29, **2019**

PhD and MTech Guidance

Ongoing PhD Students:

- Ms. Yamini Janghel
  Thesis title: *Developing an Accelerated First Principles Approach for Modelling Point-Defect Thermodynamics of Materials*
  Joined: December 2023

- Ms. Namrata Das
  Thesis title: *Developing First and Second Principles Approaches to model the effect of point defects on ferroelectric properties of oxides*
  Joined: January 2025

Graduated MTech Students:

- Mr. Sivavenkatesh R (2023 – 2025)
  Thesis title: *Computational Modeling of Disordered Alloys*
  Current Affiliation: Senior Engineer, Scandisk, Bangalore, India

- Mr. Rishabh Shukla (2023 – 2025)
  Thesis title: *A Density Functional Theory Based Study of Zr and Gd Doped HfO_2*
  Current Affiliation: Sr Engineer Integration & Yield, GlobalFoundaries, Bangalore, India

- Ms. Jyoti Chaudhary (2022 – 2024)
  Thesis title: *Computational Modeling of Stacking Fault Energy in Nickel and Nickel-based Alloys*
  Current Affiliation: PhD student at IISc, Bangalore, India

Code Development

- `https://github.com/ajgoyal/pylada_defects`
  Lead developer of **Pylada-Defects** a code for automating first principles density functional theory (DFT)-based point defect calculations

- `https://github.com/PV-Lab/SPProC`
  Contributed high-throughput DFT data for the development of **SPProC** a physics informed machine learning tool for optimizing perovskite stability

Selected Academic and Administrative Services

- Reviewed (ORCID: 0000-0001-5991-9562) articles for journals npj Computational Materials, APL Materials, Chemistry of Materials, Computational Materials Science, Journal of Applied Physics, ACS Applied Energy Materials

- Faculty advisor, Materials Science and Metallurgical Engineering 2023 B.Tech. students

- Faculty advisor, Computational Engineering 2023 B.Tech. students

- Member of the MSME Department Curriculum, and Faculty Search Committees