

# Anuj Goyal

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<b>Contact</b>	<b>Assistant Professor</b> Materials Science & Metallurgical Engineering, Indian Institute of Technology (IIT), Hyderabad Kandi - 502284, Sangareddy Telangana, India	Office: MSME 204 +91 63988 33633 <a href="mailto:anujgoyal@msme.iith.ac.in">anujgoyal@msme.iith.ac.in</a> <a href="#">LinkedIn</a> , <a href="#">Google Scholar</a>
<b>Profile</b>	I employ first-principles computational modeling and machine learning techniques to characterize and predict properties of materials for electronics, computing, and energy applications  <b>Research interests</b> in computational materials discovery and design, metals and semiconductors (oxides, nitrides, chalcogenides, halides), electronic structure theory, defect physics and thermodynamics, multi-scale modeling	
<b>Employment</b>	<b>Assistant Professor</b> Materials Science & Metallurgical Engineering, <b>Indian Institute of Technology, Hyderabad</b> Kandi - 502284, Sangareddy	<b>Dec. 2022 – present</b>
	<b>Research Scientist II</b> Theory and Computation, Materials Physics Group, <b>National Renewable Energy Laboratory</b> , Golden, CO 80401 Advisor: <a href="#">Dr. Stephan Lany</a> , Sr. Scientist	<b>Nov. 2019 – Aug. 2022</b>
	<b>Postdoctoral Fellow</b> Department of Metallurgy and Materials Engineering, <b>Colorado School of Mines</b> , Golden, CO 80401 Advisor: <a href="#">Prof. Vladan Stevanović</a>	<b>April 2016 – Oct. 2019</b>
	<b>Postdoctoral Associate</b> Department of Materials Science and Engineering, <b>University of Florida</b> , Gainesville, FL 32611 Advisor: <a href="#">Prof. Simon R. Phillpot</a>	<b>Sept. 2015 – March 2016</b>
<b>Education</b>	<b>Ph.D., Materials Science and Engineering</b> , <b>University of Florida</b> , Gainesville, FL 32611 Dissertation: <a href="#">Multiscale computational modeling of defects in uranium dioxide</a> Advisor: <a href="#">Prof. Simon R. Phillpot</a>	<b>2011 – 2015</b> GPA: 4.0/4.0
	<b>M.S., Materials Science and Engineering</b> , <b>University of Florida</b> Gainesville, FL 32611	<b>2010 – 2012</b> GPA: 4.0/4.0
	<b>B.Tech. &amp; M.Tech., Metallurgical and Materials Engineering</b> , <b>Indian Institute of Technology, Madras</b> Chennai - 600036, India	<b>2005 – 2010</b> GPA: 8.6/10.0

**Publications**    **2 under review, 18 published, and 4 in preparation**

([Google Scholar](#): H-index = 13, Total citations ~ 855)

**Manuscript under review:**

1. M. Witman\*, **A. Goyal\***, T. Ogitsu, A. H. McDaniel, and S. Lany, “[Graph neural network modeling of vacancy formation enthalpy for materials discovery and its application in solar thermochemical water splitting](#)”, under review *Nature Computational Science* **2022**. DOI:10.26434/chemrxiv-2022-frcns. (\*authors contributed equally.)
2. 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  \$\text{BaCe}\_{0.25}\text{Mn}\_{0.75}\text{O}\_{3-\delta}\$  Before and After Thermal Reduction](#)”, under review *Chemistry of Materials* **2022**. ArXiv:2209.13267

**Published:**

3. N. A. Strange, J. Park, **A. 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<sub>3</sub>Ce<sub>0.75</sub>Mn<sub>2.25</sub>O<sub>9</sub> during thermochemical reduction of 12R-Ba<sub>4</sub>CeMn<sub>3</sub>O<sub>12</sub>:Identification of a polytype in the Ba\(Ce,Mn\)O<sub>3</sub> family](#)”, *Inorganic Chemistry* **61**, 16, 6128-6137 **2022**. DOI: 10.1021/acs.inorgchem.2c00282. Impact factor (IF) = 5.16
4. **A. Goyal**, A. Zakutayev, V. Stevanović and S. Lany, “[Computational Fermi level engineering and doping-type conversion of Mg:Ga<sub>2</sub>O<sub>3</sub> via three-step synthesis processing](#)”, *Journal of Applied Physics* **129**, 245704 **2021**. DOI: 10.1063/5.0051788. IF = 2.55
5. S. Sun, A. Tiihonen, F. Oviedo, Z. Liu, J. Thapa, N. T. P. Hartono, **A. 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. IF = 15.59
6. **A. 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. IF = 3.30
7. **A. 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. IF = 9.81
8. P. Gorai, **A. 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. IF = 12.73
9. **A. Goyal**, K. Mathew, R. G. Hennig, A. Chernatynskiy, C. R. Stanek, S. T. Murphy, D. A. Anderson, S. R. Phillpot and B. P. Uberuaga, “[The conundrum of relaxation volumes in first-principles calculations of charge defects in UO<sub>2</sub>](#)”, *Applied Sciences* **9** (24), 5276 **2019**. DOI: 10.3990/app9245276. IF = 2.68
10. J. Male, M. T. Agne, **A. 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. IF = 13.27

11. L. T. Schelhas, Z. Li, J. A. Christians, **A. 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. IF = 38.53
12. **A. Goyal**, and V. Stevanović, “[Metastable rocksalt ZnO is p-type dopable](#)”, *Physical Review Materials* 2, 084603 **2018**. DOI:10.1103/PhysRevMaterials.2.084603. IF = 3.99
13. **A. 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. IF = 9.81
14. **A. 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. IF = 13.20
15. **A. 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**. IF = 3.30
16. S. A. Miller, P. Gorai, B. R. Ortiz, **A. 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. IF = 9.81
17. Y. Li, **A. 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. IF = 5.23
18. **A. 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. IF = 4.04
19. K. Choudhary, T. Liang, A. Chernatynskiy, Z. Lu, **A. 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. IF = 2.33
20. **A. 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. IF = 2.94

#### Manuscripts in preparation:

21. **A. Goyal**, M. Sanders, R. O’ Hayre, and S. Lany, “Thermodynamic model for repulsive defect interactions in off-stoichiometric  $\text{Sr}_{1-x}\text{Ce}_x\text{MnO}_3$ ”. In preparation.
22. **A. Goyal**, and S. Lany, “Electronic structure and thermodynamic defects modeling of  $\text{Ba}_4\text{XMn}_3\text{O}_{12}$  (X=Nb,Ce,Pr) oxides for solar thermochemical hydrogen production”. In preparation.
23. **A. Goyal**, A. Zakutayev, and V. Stevanović, “Rocksalt ZnO, a promising transparent, high-mobility, and ambipolar semiconductor”, In preparation.

24. Ximeng Wang, **Anuj Goyal**, Peng Zhou, Juan C. Nino, Jonathan Scheffe, Stephan Lany, Simon R. Phillpot, “Doped LaMnO<sub>3</sub> for water splitting by density functional theory calculations”, In preparation.

#### Honors & Awards

**Key Contributor Award**, Materials Physics Group, MCCS Directorate, NREL, 2021  
**Research work highlighted** at the Center for Next Generation of Materials Design, NREL, 2017  
**Best Poster Presentation Award**, The Minerals, Metals and Materials Society (TMS), 2015  
**Outstanding International Graduate Student Award**, University of Florida, 2014  
Awarded **Membership, Tau Beta Pi**, Engineering Honor Society, 2014  
Awarded **Scholarship for MEV Summer School** at Oak Ridge National Laboratory, 2012  
Awarded **Certificate of Outstanding Achievement**, University of Florida, 2011-14 (won 4 times)  
Awarded **Graduate Aptitude in Engineering Scholarship** at IIT Madras, India, 2009

#### Invited Talks

“Point Defects Modeling to Accelerate Materials Discovery in Solar Thermochemical Water Splitting”, **Indian Institute of Technology (IIT), Gandhinagar**, Gujarat, India, September 20, **2022**

“Point Defects Modeling to Accelerate Materials Discovery in Solar Thermochemical Water Splitting”, **Indian Institute of Technology (IIT), Hyderabad**, Telangana, India, July 12, **2022**

“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, July 29, **2019**

“Computationally guided design of materials”, **Los Alamos National Laboratory (LANL)**, Los Alamos, NM, April 16, **2018**

“Multiscale computational modeling of defects in uranium dioxide”, **National Renewable Energy Laboratory (NREL)**, Golden, CO, January 22, **2016**

#### Conferences

##### Selected contributed talks:

**A. Goyal**, S. Bauers, and S. Lany, “Instability of rock-salt cubic NbN in density functional calculations”, **APS March Meeting**, March 17 **2022**

**A. Goyal**, M. Sanders, R. O’Hayre, and S. Lany, “Computational defect and thermodynamic modeling of redox behavior of complex oxides for solar thermochemical hydrogen (STCH) production”, **MRS Fall Meeting**, Online, December 8 **2021**

**A. Goyal**, A. Zakutayev, V. Stevanović and S. Lany, “Computational fermi level engineering and doping-type conversion of Ga<sub>2</sub>O<sub>3</sub> via three-step processing”, **APS March Meeting**, Online, March 17 **2021**

**A. Goyal**, A. Zakutayev, and V. Stevanović, “Ambipolar doping of rocksalt ZnO”, **30<sup>th</sup> International Conference on Defects in Semiconductors**, Seattle, WA, July 23, **2019**

**A. Goyal**, Paul Kairys and V. Stevanović, “Understanding site-specific contributions to phase stability and band gap in hybrid perovskite”, **European MRS Spring Meeting**, Nice, France, May 27, **2019**

**A. Goyal**, Paul Kairys and V. Stevanović, “Understanding site-specific contributions to phase stability and band gap in hybrid perovskite”, **MRS Spring Meeting**, Phoenix, AZ, April 4, **2018**

**A. Goyal**, P. Gorai, H. Peng, S. Lany and V. Stevanović, “A computational framework for automation of point defect calculations”, **APS March Meeting**, New Orleans, LA, March 13, **2017**

**A. Goyal**, A. Chernatynskiy, G. Subramanian, D. A. Andersson, B. P. Uberuaga and S. R. Phillpot, “Sensitivity analysis and uncertainty quantification in a multi-scale model for defect diffusion under arbitrary strain fields”, **MRS Spring Meeting**, Phoenix, AZ, March 31, **2016**

**A. Goyal**, T. Rudzik, B. Deng, M. Hong, A. Chernatynskiy, S. B. Sinnott and Simon R. Phillpot, “Segregation of fission products to edge dislocations in uranium dioxide”, **MRS Fall Meeting**, Boston, MA, December 3, **2013**

**Selected poster presentations:**

**A. Goyal**, and V. Stevanović, “Metastable rocksalt ZnO is p-type dopable”, **Gordon Research Conference (GRC) on Defects in Semiconductors**, New London, NH, August 19 - 24, **2018**

**A. Goyal**, G. Subramanian, D. A. Andersson, C. R. Stanek, S. R. Phillpot and B. P. Uberuaga, “Atomistic characterization of uranium vacancy interaction with external strains in UO<sub>2</sub>”, **TMS Annual Meeting**, Orlando, FL, **2015**, (*Won the best poster presentation award*)

**Skills**

**Electronic Structure Codes:** VASP, Quantum-ESPRESSO, QUESTAAL

**Molecular Dynamics Codes:** LAMMPS, GULP

**Programming:** Python, FORTRAN, Mathematica, GNU Octave, Bash

**Computational Materials Tools:** ATAT, Pylada, Pymatgen, ASE

**GitHub Projects:**

- Lead developer of [Pylada-Defects](#) a code for automating first principles point defect calculations
- Contributor to [SPProC](#) a physics informed machine learning tool for optimizing perovskite stability

**Academic Service**

**Reviewed** articles for journals ([ORCID: 0000-0001-5991-9562](#)):

- npj Computational Materials
- Chemistry of Materials
- Journal of Physical Chemistry Letters
- Journal of Materials Science
- APL Materials
- Journal of Physical Chemistry C
- Computational Materials Science
- Journal of Applied Physics

**References**

**Dr. Stephan Lany**

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**Prof. Simon. R. Phillpot**

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Vladimir A. Grodsky Professor of Materials Science and Engineering,  
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