Christopher A. Sutton

☎ 501.258.4098
✉ cs113@mailbox.sc.edu

Assistant Professor | Department Chemistry and Biochemistry | University of South Carolina

RESEARCH SUMMARY

My research is focused on developing and applying first-principles calculations combined with machine-learning methods to design, predict, and understand new and functional materials.

APPOINTMENTS

Assistant Professor
University of South Carolina, Columbia, SC — 2021 – Present

PROFESSIONAL PREPARATION

Postdoctoral Researcher, Advisor: Matthias Scheffler
Fritz Haber Institute of the Max Planck Society, Berlin, DE — 2015 – 2020

Postdoctoral Researcher, Advisor: Weitao Yang
Duke University, Durham, NC — 2014 – 2015

Graduate Research Assistant, Advisor: Jean-Luc Brédas
Georgia Institute of Technology, Atlanta, GA — 2009 – 2014

FELLOWSHIPS AND AWARDS

- Alexander von Humboldt Postdoctoral Fellowship — Sept. 2016 – Sept. 2018
- 67th Lindau Nobel Laureate Meeting Attendee (Chemistry) — 2017
- BAEF Fellowship (declined) — 2014
- GT Chemistry and Biochemistry Outstanding Graduate Student Service Award — Nov. 2013
- Graduate Presidential fellowship recipient at Georgia Tech — Aug. 2009 – May 2013
- Undergraduate Presidential scholarship recipient at UCA — Aug. 2004 – May 2008

SERVICE (Since joining USC)

5 Co-organized symposium *Emerging Energy Applications of Low-Dimensional Layered and Crystalline Materials* at Fall MRS Meeting — Dec. 2023
4 Co-organized SETCA 2023 (www.setca2023.com) at USC — May 2023
3 Co-organized session in computational catalysis at annual meeting for Spring ACS meeting — March 2022
2 Organized sessions at annual meeting for the Big Data for Health Center at USC — Feb. 2022 and 2023
1 Served on the steering committee for the Big Data for Health center at USC — Aug. 2021 – Present

FUNDING AT USC

9 DOE/HFTO *in negotiations* (co-PI; Total award amount: $1,000,000) — Sept. 2023 – Aug. 2026
Accelerated Discovery and Demonstration of Advanced Perovskites for Efficient Solar Thermochemical Hydrogen Production

8 NSF EPSCoR RII Track 1 program OIA-2242812 (co-PI; Total award amount: $20,000,000) — June 2023 – July 2028
ADAPT in SC: AI-enabled Devices for the Advancement of Personalized and Transformative healthcare in South Carolina

7 DOD/DEPSCOR 23RT0398 (PI; Total award amount: $600,000) — Aug. 2023 – July 2026
Unraveling the Role of Cation Solvation in Aqueous Zn-Ion Batteries: A Combined Theoretical and Experimental Approach

6 DOE/BES DE-SC0023377 (co-PI; Total award amount: $2,550,000) — Oct. 2022 – Sept. 2025
Understanding the Role of Defects to Accelerate Wadsley-Roth Niobates for Long-Duration Energy Storage

5 USC ASPIRE II (co-PI; Total award amount: $100,000) — Aug. 2022 – Sept. 2023
Discover New Cubic Superionic Conductors beyond Traditional Perovskite Structures

4 DOE/ SETO DE-EE0009515 (co-PI; Total award amount: $1,200,000) Oct. 2021 – Sept. 2024
Accelerated Selection of Optimal Perovskite Alloys for Solar PV using a Combined Quantum and Machine Learning Hierarchical Approach

3 DOE/CCS DE-SC0022247 (co-PI; Total award amount: $2,900,000) Sept. 2021 – Aug. 2025
Beyond-DFT Electrochemistry with Accelerated and Solvated Techniques (BEAST)

2 SC EPSCOR GEAR Award (PI; Total award amount: $60,000) March 2021 – Feb. 2022
Data driven optimization of the electrolyte composition for improving cycling stability in rechargeable Li-based batteries

1 AFOSR/EOARD 20IOE044 (Total award amount: $200,000) March 2021 – Feb. 2024
Machine-Learning Aided Screening of Organic-Inorganic Perovskites as Efficient Photoabsorbers

PUBLICATIONS AT USC

31 RP Xian, R Morelock, I Hadar, C Musgrave, **C Sutton*** "From Structure Mining to Unsupervised Exploration of Atomic Octahedral Networks", *Submitted, 10.26434/chemrxiv-2023-n6p86,* 2023.

30 K Fazel, N Karimitari, T Shah, **C Sutton***, R Sundararaman* "Improving the Reliability of Machine Learned Potentials for Modeling Inhomogeneous Liquids", *Submitted, http://arxiv.org/abs/2306.00970,* 2023.

29 S Adhikari, CJ Bartel, **C Sutton*** "Interpretable Machine Learning to Understand the Performance of Semi-local Density Functionals for Materials Thermochemistry", *Phys. Rev. B (under review),* 2023.

28 C Tezak, N Singstock, A Alherz, D Vigil-Fowler, **C Sutton**, R Sundararaman, C Musgrave "Revised Nitrogen Reduction Scaling Relations from Potential-Dependent Modeling of Chemical and Electrochemical Steps", *ACS Catal. (under review), 10.26434/chemrxiv-2023-v73sk*, 2023.

27 S Adhikari, J Clary, R Sundararaman, C Musgrave, D Vigil-Fowler, **C Sutton*** "Accurate Prediction of HSE06 Band Structures for a Diverse Set of Materials Using Δ-learning", *Chem. Mater. (under review), 10.26434/chemrxiv-2023-n6p86,* 2023.

26 W Baldwin, X Liang, J Klarbring, M Dubajic, D Dell'Angelo, **C Sutton**, C Caddeo, SD Stranks, A Mattoni, A Walsh, G Csanyi "Dynamic Local Structure in Cesium Lead Iodide: Spatial Correlation and Transient Domains", *Small (under review),* 2023.

25 M Wells, J Hempel, S Adhikari, Q Wang, D Allen, A Costello, C Bowen, S Parkin, **C Sutton**, and AJ Huckaba, "Structure and Piezoelectricity Due to B Site Cation Variation in ABn+Cln+2 Hybrid Histammonium Chlorometallate Materials", *Inorg. Chem.*, 61, 44, 17746–17758, 2022.

24 L Foppa, **C Sutton**, L Ghiringhelli, S De, P Löser, S Schunk, A Schaefer, M Scheffler, "Learning design rules for selective oxidation catalysts from high-throughput experimentation and artificial intelligence" *ACS Catal.*, 12, 4, 2223–2232, 2022.

23 NR Singstock, JC Ortiz-Rodríguez, JT Perryman, **C Sutton**, Jesús M. Velázquez, and CB Musgrave "Machine Learning Guided Synthesis of Multinary Chevrel Phases for Tunable Energy Materials", *J. Am. Chem. Soc.*, 143, 9113−9122, 2021.

22 **C Sutton*** and S Levchenko "Review: First-Principles Atomistic Thermodynamics and Configurational Entropy", Frontiers in Chemistry, 8, 2020.

PUBLICATIONS PRIOR TO USC

21 C Wouters, **C Sutton**, LM Ghiringhelli, T Markurt, R Schewski, A. Hassa, H. von Wenckstern, M. Grundmann, M Scheffler, M Albrecht, "Investigating the ranges of (meta)stable phase formation in $(In_xGa_{1-x})_2O_3$: Impact of the cation coordination" *Phys. Rev. Mater.*, 4, 125001, 2020.

20 **C Sutton**,* M Boley,* LM Ghiringhelli, M Rupp, J. Vreeken, M Scheffler "Identifying Domains of Applicability of Machine Learning Models for Materials Science", *Nat. Commun.*, 11, 1-9, 2020.

19 CJ Bartel, JM Clary, **C Sutton**, D Vigil-Fowler, BR Goldsmith, AM Holder, CB Musgrave, "Computational Discovery of Cesium Chloride Double Perovskite Optoelectronic Materials", *J. Am. Chem. Soc.,* 142, 11, 5135-5145, 2020.

18 **C Sutton***, et al. "Crowd Sourcing Materials Science Challenges with the NOMAD 2018 Kaggle Competition" *npj Comput. Mater.* 5, 111, 2019.

17 CJ Bartel, **C Sutton**, B. R. Goldsmith, R Ouyang, CB Musgrave, LM Ghiringhelli, M Scheffler "New Tolerance Factor for the Prediction of Perovskite Oxides and Halides" *Science Advances*, 5, 2, 2019.

16 BR Goldsmith, J Esterhuizen, J-X Liu, CJ Bartel, **C Sutton** "Perspective: Machine Learning for Heterogeneous Catalyst Design and Discovery" *AIChe Journal*, 64, 2311, 2018.

15 R Al-Saadon, **C Sutton**, W Yang "Accurate Treatment of Charge-Transfer Excitations and Thermally Activated Delayed Fluorescence Using the Particle-particle Random Phase Approximation" *J. Chem. Theory Comput.*, 14, 3196, 2018.

14 **C Sutton**, Y Yang, D Zhang, W Yang "Single, Double Electronic Excitations and Exciton Effective Conjugation Lengths in π-conjugated Systems" *J. Phys. Chem. Lett.*, 9, 4029, 2018.

13 **C Sutton**, NR Tummala, T Kemper, SG Aziz, JS Sears, V Coropceanu, JL Brédas "Understanding the Effects of Electronic Polarization and Delocalization on Charge-Transport Levels in Oligoacene Systems" *J. Chem. Phys.*, 146, 224705, 2017.

12 **C Sutton**,* NR Tummala, D Beljonne, JL Brédas "Singlet Fission in Rubrene Derivatives: Impact of Molecular Packing" *Chem. Mater.*, 29, 2777, 2017.

11 **C Sutton**, C Risko, JL Brédas "Review: Non-Covalent Intermolecular Interactions in Organic Electronic Materials: Implications for Molecular Packing and Electronic Properties" *Chem. Mater.,* 28, 3, 2016 (Front cover).

10 NR Tummala, **C Sutton**, C Risko, JL Brédas "Solvent and Solvent Additive Effects on Aggregation of PCBM: A Molecular Perspective" *Chem. Mater.*, 27, 8261, 2015.

9 **C Sutton**, MS Marshall, CD Sherrill, C Risko, JL Brédas "Rubrene: The Interplay Between Intramolecular and Intermolecular Interactions Determines the Planarization of Its Tetracene Core in the Solid State" *J. Am. Chem. Soc.*, 137, 8775, 2015.

8 A Fonari, **C Sutton**, V Coropceanu, JL Brédas "The Impact of Exact Exchange Energy in the Description of the Electronic Structure of Organic Charge Transfer Molecular Crystals" *Phys. Rev. B*, 90, 165205, 2014.

7 **C Sutton**, T Körzdörfer, MT Gray, M Brunsfeld, RM Parrish, CD Sherrill, JS Sears, JL Brédas, "Accurate Description of Torsion Potentials in Conjugated Polymers using Density Functionals with Reduced Self-interaction Error" *J. Chem. Phys.*, 140, 054310, 2014.

6 **C Sutton**, T Körzdörfer, V Coropceanu, JL Brédas "Towards a Robust Quantum-Chemical Description of Organic Mixed-Valence Systems" *J. Phys. Chem. C*, 118, 3925, 2014.

5 PJ Diemer, CR Lyle, Y Mei, **C Sutton**, MA Loth, JE Anthony, V Coropceanu, JL Brédas, OD Jurchescu, "Vibration-Assisted Crystallization Improves Organic/Dielectric Interface in Organic Thin-Film Transistors" *Adv. Mater.,* 25, 6956, 2013 (Back cover). Highlighted in Nature and Nature Materials.

4 KA McGarry, W Xie, **C Sutton**, C Risko, Y Wu, V Young, JL Brédas, CD Frisbie, CJ Douglas "Rubrene-Based Single-Crystal Organic Semiconductors: Synthesis, Electronic Structure, and Charge-Transport Properties" *Chem. Mater.*, 25, 2254, 2013.

3 **C Sutton**, JS Sears, V Coropceanu, JL Brédas "Understanding the Density Functional Dependence of DFT-Calculated Electronic Couplings in Organic Semiconductors" *J. Phys. Chem. Lett.*, 4, 919, 2013.

2 PJ Desrochers, **CA Sutton**, ML Abrams, S Ye, F Neese, J Telser, A Ozarowski, J Krzystek "Electronic Structure of Nickel(II) and Zinc(II) Borohydrides from Spectroscopic Measurements and Computational Modeling" *Inorg. Chem.,* 51, 2793, 2012.

1 T Körzdörfer, JS Sears, **C Sutton**, JL Brédas "Long-Range Corrected Hybrid Functionals for π-Conjugated Systems: Dependence of the Range-Separation Parameter on Conjugation Length" *J. Chem. Phys.*, 135, 204107, 2011.