# Christopher A. Sutton

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## RESEARCH SUMMARY

My research is focused on developing and applying computational approaches such as density functional theory combined with machine-learning methods to design, predict, and understand new and functional materials.

## EDUCATION

***Postdoctoral Researcher***, May 2015 – 2020
Fritz Haber Institute of the Max Planck Society
Advisor: Matthias Scheffler

***Postdoctoral Researcher***, Nov. 2014 – May 2015
Duke University
Advisor: Weitao Yang

***Physical Chemistry (Ph.D.)***, Aug. 2009 – Nov. 2014
Georgia Institute of Technology
Advisor: Jean-Luc Brédas

***Chemistry (B.S.)***, Aug. 2004 – May 2008
University of Central Arkansas

## FELLOWSHIPS AND AWARDS

- Alexander von Humboldt Postdoctoral Fellowship — September 2016 – September 2018
- 67th Lindau Nobel Laureate Meeting Attendee (Chemistry) — 2017
- BAEF Fellowship (declined) — 2014
- GT Chemistry and Biochemistry Outstanding Graduate Student Service Award — November 2013
- Graduate Presidential fellowship recipient at Georgia Tech — August 2009 – May 2013
- Undergraduate Presidential scholarship recipient at UCA — August 2005 – May 2008

## PUBLICATIONS

20 **C Sutton**, M Boley, LM Ghiringhelli, M Rupp, J. Vreeken, M Scheffler "Identifying Domains of Applicability of Machine Learning Models for Materials Science", *Nature Communications*, 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", JACS, 2020.

18 **C Sutton**, et al. "Crowd Sourcing Materials Science Challenges with the NOMAD 2018 Kaggle Competition" npj Computational Materials 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" Journal of Chemical Theory and Computation, 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" The Journal of Physical Chemistry Letters, 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" The Journal of Chemical Physics 146, 224705, 2017.

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12 **C Sutton**, NR Tummala, D Beljonne, JL Brédas "Singlet Fission in Rubrene Derivatives: Impact of Molecular Packing" Chemistry of Materials 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" Chemistry of Materials, 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" Chemistry of Materials, 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" Journal of the American Chemical Society, 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" Physical Review 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" Journal of Chemical Physics, 140, 054310, 2014.

6 **C Sutton**, T Körzdörfer, V Coropceanu, JL Brédas "Towards a Robust Quantum-Chemical Description of Organic Mixed-Valence Systems" Journal of Physical Chemistry 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" Advanced Materials, 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" Chemistry of Materials, 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" The Journal of Physical Chemistry Letters, 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" Inorganic Chemistry, 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" Journal of Chemical Physics, 135, 204107, 2011.