# COMPUTING & MATERIALS FRONTIERS

**Lars C. Grabow**

*Ph.D. – University of Wisconsin*
*Dan Luss Professor, William A. Brookshire Department of Chemical and Biomolecular Engineering*
*Professor, Chemistry*

Dr. Grabow leads the Computational Catalysis and Surface Chemistry group at UH. He is the first recipient of the Dan Luss Endowed Professorship and was elected into the 2018 Class of Influential Researchers by Industrial & Engineering Chemistry (I&EC) Research. He was awarded the NSF CAREER (2015) and DOE Early Career Awards (2014), and was recognized by the University of Houston with the Teaching Excellence Award (2014), Excellence in Research, Scholarship or Creative Activity Award (2017), and the Undergraduate Research Mentoring Award (2020). His group uses the state-of-the-art high-performance computing facilities at the UH Hewlett Packard Enterprise Data Science Institute and at the national supercomputing centers to design solid state materials with functional interfaces. Dr. Grabow's research can be applied to environmental catalysis, carbon-neutral energy production, hydrocarbon chemistry, and electrochemical energy storage devices. Additional information regarding the research conducted by Dr. Grabow's group is available at ***https://youtu.be/_wZLKunnxfU.***

## COMPUTATIONAL MATERIAL DESIGN

High performance, functional materials are a cornerstone for advanced manufacturing and innovative technologies. In particular, the Houston area is home to many chemical manufacturers who use catalytic materials to intensify their processes by making them more efficient, selective and less resource consuming. Catalysts are also used to treat vehicle exhaust, treat waste water and enable renewable energy technologies. The electrification of transportation, and in the long term, possibly the chemical industry, may also require innovative and safe electrochemical storage solutions.

Dr. Grabow's group integrates physical models with machine learning approaches to develop computational tools that help in discovering and designing novel catalysts with tailored properties and solid-state electrolytes for safer batteries. Dr. Grabow conducts transient kinetic experiments in a Temporal Analysis of Products (TAP) reactor to validate model predictions. Designing novel materials in silico is an exciting avenue that aligns well with the mulit-agency Materials Genome Initiative and current interests to leverage artificial intelligence for data-driven material discoveries that avoid costly trial-and-error experimentation. A recent example of a computational catalyst discovery is a new cost-effective metal alloy catalyst designed for diesel exhaust treatment, for which laboratory experiments show high CO oxidation activity below 150°C and no inhibition by other pollutants.

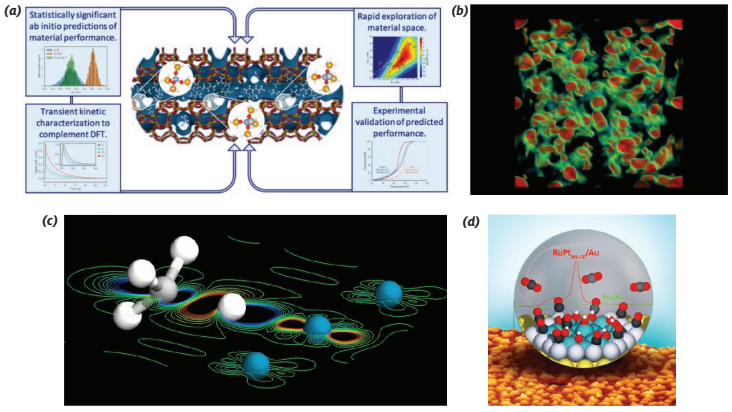


***Figure (a)*** *is a graphical schematic of the research activities in Dr. Grabow's laboratory.* ***Figure (b)*** *shows the electron density of a hypothetical new material for battery applications generated by a machine learning algorithm.* ***Figure (c)*** *shows the electron density change in methane during its activation over a palladium catalyst.* ***Figure (d)*** *shows the CO electro-oxidation activity of Pt-decorated Ru nanoclusters.*

***Selected Publications***

*1. Rao, K. K.; Do, Q. K.; Pham, K.; Maiti, D.; Grabow, L. C. Extendable Machine Learning Model for the Stability of Single Atom Alloys. Top. Catal. 2020, 1 (0123456789), 3.*

*2. Rao, K. K.; Yao, Y.; Grabow, L. C. Accelerated Modeling of Lithium Diffusion in Solid State Electrolytes Using Artificial Neural Networks. Adv. Theory Simulations 2020, 2000097, 2000097.*

*3. Thirumalai, H.; Rimer, J. D.; Grabow, L. C. Quantification and Statistical Analysis of Errors Related to the Approximate Description of Active Site Models in Metal-Exchanged Zeolites. ChemCatChem 2019, 11 (20), 5055–5067.*

*4. Song, Y.; Grabow, L. C. Activity Trends for Catalytic CO and NO Co-Oxidation at Low Temperature Diesel Emission Conditions. Ind. Eng. Chem. Res. 2018, 57 (38), 12715–12725.*

*5. Goulas, K. A.; Sreekumar, S.; Song, Y.; Kharidehal, P.; Gunbas, G.; Dietrich, P. J.; Johnson, G. R.; Wang, Y. C.; Grippo, A. M.; Grabow, L. C.; et al. Synergistic Effects in Bimetallic Palladium–Copper Catalysts Improve Selectivity in Oxygenate Coupling Reactions. J. Am. Chem. Soc. 2016, 138 (21), 6805–6812.*

*6. Nelson, R. C.; Baek, B.; Ruiz, P.; Goundie, B.; Brooks, A.; Wheeler, M. C.; Frederick, B. G.; Grabow, L. C.; Austin, R. N. Experimental and Theoretical Insights into the Hydrogen-Efficient Direct Hydrodeoxygenation Mechanism of Phenol over Ru/TiO2. ACS Catal. 2015, 5 (11), 6509–6523.*

*7. Saavedra, J.; Doan, H. A.; Pursell, C. J.; Grabow, L. C.; Chandler, B. D. The Critical Role of Water at the Gold-Titania Interface in Catalytic CO Oxidation. Science 2014, 345, 1599–1602.*

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