CASE STUDY

De Novo Design of Hole-Conducting Molecules for Organic Electronics

Panasonic and Schrödinger scientists designed over 50 novel molecules with improved hole mobility by performing large-scale density functional theory (DFT) calculations and machine learning inverse design.

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Executive Summary

Tremendous Time Saved and Cost Reduced

- 3 *de novo* design methods developed and assessed
- 14 million molecules enumerated and screened
- 9,000 DFT calculations performed
- Over 50 molecules identified with target performance profile

Performance Improved

Identified molecules with lower hole reorganization energy (up to 22% reduction) than the lowest one in training dataset

Highly Predictive Machine Learning (ML) Models Developed

Leveraged data based on DFT calculations of 250,000 molecules

New Insights Proposed

High quality *de novo* design complements molecular enumeration and virtual screening

Charge carrier mobility is one of the most important characteristics of semiconductor materials.

Applications in printed electronics demand molecules with high mobility. Despite rapid progress toward discovery of new molecules with improved mobility, challenges persist. For example, the impact of topological shape of the molecules on the magnitude of hole mobility is not well understood for optimized molecular design, and it can be extremely costly and time-consuming to synthesize and assess every candidate molecule. Atomic simulations and machine learning technologies can reveal novel insights which are inaccessible to experimental methods alone.

"With Schrödinger's advanced simulation tools, we were able to explore millions of molecules and target tens of potential candidates within a short period of time, which is simply unfeasible with traditional approaches. This level of computational power changes the way we innovate. Both the scientific expertise and the excellence of technology Schrödinger brings to the table give us confidence in future collaborations."

— Nobuyuki N. Matsuzawa
General Manager of Panasonic Corporation

Approach

Scientists at Panasonic are challenged to develop novel organic semiconductor materials with higher efficiency. In order to drive innovation, Panasonic teamed up with Schrödinger for *de novo* design of new molecules leveraging the computational power and expertise of Schrödinger of **high-throughput DFT calculations, machine learning/deep learning model building, and chemical enumeration.**

Phase 1

Built highly predictive machine learning models using DFT calculations of **250,000** heteroacenes, and Schrödinger's automated quantitative structure–activity relationship tool AutoQSAR/DeepChem.

Phase 2

Explored 3 *de novo* methods (Continuous, REINVENT, and JTNN). Generation of molecules minimizing hole reorganization energy were run with trained machine learning models for each method. The top 3,000 molecules for each method (**9,000** in total) were selected for downstream DFT analysis.

Phase 3

Hole reorganization energy and hole mobility of the top-ranked molecules were calculated by DFT/MD with Schrödinger Materials Science tools, and over **50** novel molecules were identified.

Results

Scientists from Panasonic and Schrödinger performed a thorough benchmark study of three *de novo* methods and identified molecular structures in the heteroacene family, which may show improved carrier transport properties.[1] Schrödinger demonstrated strong **large-scale computing capabilities** and **in-house expertise** in machine learning to develop *de novo* methods based on knowledge and literature reports, building bayesian optimizers and reward engineering.

Result

Over 50 molecules were identified to have lower hole reorganization energy than lowest data in the training set (up to 22% reduction). We expect significant enhancement in hole mobility by the reduction of the reorganization energy in the newly-designed molecules.

Result

The best scoring compound was found by the JTNN method, followed by REINVENT. However, on the whole, the REINVENT method generated the best top 1,000 molecules.

Result

Based on the findings, the scientists propose that high-quality *de novo* methods should optimize for compounds that "fill holes" in the space of the enumeration, generating highly targeted molecules.

Conclusion

Scientists from Panasonic and Schrödinger have applied three major classes of *de novo* molecular design (inverse design) methods to the challenging problem of improving charge carrier mobility in materials science. They evaluated the performance of these methods via large-scale DFT calculation of hole reorganization energy. These methods present an attractive complement to molecular enumeration and virtual screening, and recent advances in deep learning for *de novo* design have yielded promising results for the design of novel materials.

References

1. **De Novo Design of Molecules with Low Hole Reorganization Energy Based on a Quarter-Million Molecule DFT Screen**
   Gabriel Marques*, Karl Leswing, Tim Robertson, David Giesen, Mathew D. Halls, Alexander Goldberg, Kyle Marshall, Joshua Staker, Tsuguo Morisato, Hiroyuki Maeshima, Hideyuki Arai, Masaru Sasago, Eiji Fujii, and Nobuyuki N. Matsuzawa*
   J. Phys. Chem. A 2021, 125, 33, 7331–7343

About Schrödinger

Schrödinger is an industry-leading computational solutions provider for both life science and materials science, with a mission to improve human health and quality of life by transforming the way therapeutics and materials are discovered.

With the goal to accelerate the discovery and optimization of materials by leveraging a digital chemistry platform that is governed by physics-based modeling, amplified by machine learning, and optimized through team-based intelligence, Schrödinger's Materials Science solutions offer unprecedented insights into the mechanisms and properties of materials and chemical systems in a wide range of technological applications: Organic Electronics, Polymeric Materials, Consumer Packaged Goods, Catalysis & Reactive Systems, Semiconductors, Energy Capture & Storage, Complex Formulations, Metals, Alloys & Ceramics.

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