Schrödinger

6 月 4 日(火)10:00-11:00

Advancing Polymer Design and Analysis through Integrated Machine Learning and Molecular Modeling Techniques

Mohammad Atif Faiz Afzal
Principal Scientist

The use of polymers is widespread across various industries, including aerospace, electronics, and automotive, primarily due to their ease of processing and ability to impart lightness and flexibility to devices. By altering polymer chemistry, we can customize their mechanical and thermophysical properties to meet specific requirements. However, the exploration and testing of the vast chemical space in experimental setups face significant constraints. Modeling and simulation provide a quicker method for characterizing and designing new polymer materials. Integrating these modeling tools with machine learning enhances the accuracy of these characterizations and further speeds up the design cycle for new polymers. These tools are particularly valuable in industries like pharmaceuticals and consumer goods, where polymers play a crucial role in formulations, and understanding the interactions between polymers and other components is essential. Molecular modeling has proven to be an effective technique for examining these interactions and analyzing microstructure formation. In this presentation, I will present several case studies that illustrate the substantial benefits of molecular modeling and machine learning in these varied polymer applications.

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6 月 4 日(火)11:00-12:00

可視光応答型の水分解光触媒に向けた
新規チタン酸窒化物化合物の探索

シニア サイエンティスト　青木　祐太

再生可能なエネルギー源を用いた水素生産技術は, 水素エネルギー利用を持続可能なものとする上で必要不可欠である. これを実現するひとつのアプローチが, 太陽光を利用した水の光触媒分解である. TiO2 を光触媒とした水分解反応の発見以来, 数多くの物質が光触媒材料として提案されてきたが, TiO2 は構成元素の豊富さや化学的安定性の観点から, 依然として光触媒材料として大きなアドバンテージを有している.

TiO2 を水分解用の光触媒材料として用いる場合, 大きな課題となるのはそのバンドギャップの大きさである. TiO2 のバンドギャップはおよそ 3.0 eV 程度であり, 波長 400nm 以下の紫外光しか活用できない. 太陽光のエネルギーを有効活用するには可視光の活用が不可欠である. TiO2 に可視光応答性を付与するためには N ドーピングをはじめとした化学ドーピングが有効であることが示されているが, これによって与えられる可視光応答性は, TiO2 が有している紫外光に対する応答性と比べて弱いものにとどまっている.

今回の発表ではそれに代わるアプローチとして, 新たな化合物としてのチタン酸窒化物を探索する方法を提案する. ここでは前駆物質として, 組成式 TinO2n-1 (n ≥ 2)で与えられるチタン亜酸化物系を考える. Ti の最も安定な酸化状態が Ti4+であることを念頭に置くと, この組成式中の 2n-1 個の O 原子のうち, 2 個を N 原子に置き換えることで, 安定なチタン酸窒化物化合物 TinN2O2n-3 (n ≥ 2) を構成できると期待できる. この元素置換の可能なパターンを全て列挙するのは大変な作業であるが, Materials Science Suite (MSS) にはこれを自動で行う機能が搭載されている. このようにして構成した TinN2O2n-3 の各構造について, MSS 搭載の Quantum ESPRESSO パッケージでエネルギー的安定性およびバンド構造を計算した. 結果として, TinN2O2n-3 のバンドギャップは TiO2 と比べて大幅に縮小しており, 可視光を用いた水分解光触媒として適したバンド構造を有することが確認できた. また, その合成方法についてもあわせて検討する.

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6 月 5 日(水)10:00-11:00

Accelerating the innovation of next generation cosmetics and food products through computational chemistry

Haigong Liu
Senior Scientist

As regulators and consumers demand more eco-friendly cosmetic and personal care products made from sustainably-sourced ingredients, product development faces enormous challenges to deliver new products within limited time and resources. Understanding how ingredients behave in cosmetic products will be necessary to drive new development and end to end product tracing. Only chemistry and composition is required, molecular simulation provides a unique opportunity to predict product morphology, solubility and other physical properties. Complex Interfacial systems can be leveraged to understand how individual ingredients interact with biological substrates like hair and skin surfaces.

The food industry is also facing the challenges of developing healthier, tastier, and more environmentally-sustainable products. The physics-based molecular simulation is able to predict physical properties of food product formulations, processing, and packaging materials, helping food scientists and engineers to make informed decisions before embarking on costly experimental testing. Leveraging the data from realistic molecular computational models combined with existing experimental data, researchers could build machine learning models overcoming the data sparsity issue often encountered.

In this webinar, we will present Schrödinger's transformative digital solutions to address industry driven problems in the cosmetic personal care field and the development of food products.

6 月 5 日(水)11:00-12:00

データ駆動型材料研究のための計算プラットフォーム LiveDesign

ストラテジック デプロイメント マネージャー　石崎 貴志
シニア ソリューション アーキテクト　山田 淳美

企業の研究において、探索段階でのデータの記録や計算技術の活用は個人依存になる傾向があり、日常的な業務フローとして根付いていることは稀です。LiveDesign はデータ蓄積だけでなく計算技術を Web で提供することで、誰もが計算技術を活用して、効率的で高確率な研究活動を実現することを支援するプラットフォームです。本セミナーでは、有機低分子だけでなく、配合や部品情報を記録し、それらに機械学習などの計算を適用することで、効率的な材料設計ができることをご紹介します。

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6 月 5 日(水)17:00-18:00

Efficient computation of process parameters for controlling the chemistry of deposition or etch – atomic-scale mechanism, thermodynamic competition and microkinetic modelling

Simon D. Elliott
Director - Atomic level process simulation

The unique characteristic of atomic layer deposition (ALD) and atomic layer etching (ALE) is the ability to control the growth or etching away of atomic thicknesses of a target material. In this talk we present a variety of computational techniques that help us understand, control and improve these processes. The emphasis is on choosing the right technique for the research question and time available. The same computational techniques can be used to investigate other gas-surface processes, such as catalysis or sensing.

Four types of process are conceivably in competition when a metal surface is treated with any reagent or reagent-combination: continuous deposition (CVD) or etching, or self-limiting pulsed deposition (ALD) or etching (ALE). We show that thermodynamics based on density functional theory (DFT) of bulk and surfaces is a computationally-efficient approach for distinguishing between the four processes. The temperatures and pressures for crossover between the four types of process can be estimated, with the accuracy depending on how entropy, coverage and diffusion are treated. We use the example of ruthenium metal to illustrate this simulation strategy. Ru is being investigated as a possible seed layer for interconnect electroplating in the fabrication of electronic devices, as a capacitor electrode and as a heterogeneous catalyst. Low-temperature deposition allows substrate-selectivity, which can be enhanced by punctuating the process with an additional self-limiting etch step. We therefore focus on the conditions for self-limiting versus continuous processing of Ru metal, hydride, hydroxide and oxide with respect to H2 and RuO4 reagents. We point out how to balance the cost (in terms of researcher time and computer time) against the benefit that each level of calculation can offer.

In the second part of the talk, we introduce Microkinetic Modelling, a new Schrödinger capability for examining the overall kinetics of gas-surface chemistry by solving the coupled kinetic rate equations of its constituent elementary reaction steps. This allows the simulation of macroscopic parameters such as growth rate and sticking coefficient that can be experimentally measured and used as inputs for fluid dynamics simulations. We first outline the computational scheme, where elementary steps and their activation free energies have been computed with DFT. The resulting microkinetic model for alumina ALD yields measurable quantities (e.g. relative growth per cycle and sticking coefficients) as a function of temperature and pressure, which are validated against experiment. We then show results for how microkinetic modelling can be used in specific scenarios. By adding appropriate elementary steps, the model can reveal the contribution from continuous CVD-style growth under given conditions, or under what conditions ALD can be flipped over into ALE. We also show how a microkinetic model can be used to study the variation of sticking coefficient with pressure and thus account for penetration depth and conformality within high aspect ratio features.

The two cases discussed in this talk thus illustrate how atomic-scale DFT can be embedded into higher-level computational schemes for accurate and achievable prediction of the conditions and parameters for controlling chemical processes.

6 月 6 日(木)10:00-11:00

Leveraging Schrödinger's Digital Chemistry Platform for Accelerated Development of Next-Generation Battery Materials

Garvit Agarwal
Scientific Lead, Energy Storage
Materials Science Group

The rapid advancements in rechargeable Li-ion battery (LIB) technology over the last decade has revolutionized several key industries such as transportation and consumer electronics. However, new battery chemistries are needed to meet the rapidly growing demand and to improve the power density, safety, reliability, and lifetime of LIBs. Molecular modeling has become an integral part of the design cycle of new battery chemistries. Accurate atomic scale modeling enables rapid evaluation and screening of large chemical and material design space thereby, helping industries reduce the time required to bring the new technology to the market.

In this webinar, we will discuss case studies demonstrating the impact of Schrödinger's advanced digital chemistry platform on accelerating the design and formulation of next-generation battery materials with improved properties. We will discuss the application of both physics-based and machine learning techniques for calculating key material properties and for developing structure-property relationships for the different components of batteries including electrodes, electrolytes and electrode-electrolyte interfaces. We will also introduce Schrödinger's automated active learning framework for the development of accurate machine learning force fields for calculating bulk properties of electrolytes, inorganic cathode coating materials and for modeling interfacial degradation of electrolytes.

Key Learning Objectives:

- Understand predictive capabilities of physics-based modeling for battery materials
- Learn how Schrödinger's automated high throughput simulation workflows enable rapid screening of new battery material candidates
- Application of advanced machine learning force fields for accurate modeling of electrolyte materials, cathode coatings and interfaces

6 月 6 日(木)11:00-12:00

全固体電池の負極保護膜についての解析

シニア サイエンティスト　井本 文裕

リチウムイオン電池（Lithium Ion Battery: LIB）は 1990 年代前半の商用化以降、電子機器を中心に広く使用され、既に電気自動車用電池としても市販されています。従来の有機電解液を用いる LIB には安全性や低エネルギー密度などの欠点があり、近年では不燃性固体電解質と Li 負極を利用した全固体電池が注目されています。ところが全固体電池には、（1）Li 負極からの電子移動による固体電解質の還元劣化、（2）Li 負極からの Li デンドライト成長といった問題点があります。そこで、固体電解質の還元劣化と Li デンドライト成長を防ぐために、Li 負極上に BN などの保護膜を形成することが試みられています。

本セミナーでは、Li 負極保護膜として ZnO、BN、LiCl に注目し、(a) Li 負極と保護膜の界面、(b) 保護膜と Li1.3Al0.3Ti1.7(PO4)3 (LATP)電解質の界面について、電子状態および Li が保護膜から Li 負極へ移動する障壁を第一原理的に解析した事例をご紹介いたします。計算には、Materials Science Suite（MSS）に含まれる Quantum ESPRESSO（QE）を利用いたします。Li 移動障壁の計算では、QE の一機能である Nudged Elastic Band 法（NEB 法）を利用いたします。MSS の NEB 法では、弊社にて実装を改良したスキームによる並列化効率の高い計算が可能です。

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6 月 7 日(金)10:00-11:00

Automated Digital Prediction of Chemical Degradation Products

Pavel A. DUB

Senior Principal Scientist

Chemical degradation is the process by which chemical substances undergo structural changes, leading to the breakdown of their molecular integrity into simpler chemical compounds. This process is at the heart of chemical failure and material lifetime, natural degradation and aging, and recycling. It unfolds through diverse mechanisms, among which thermal decomposition, photolysis, oxidation, and hydrolysis are the most prevalent.

The automated prediction of chemical degradation products, or degradants, for small molecules has long posed a challenge for computational chemistry, but could broadly benefit a range of industrial use cases. These include pharmaceutical ingredient degradation, disposal of chemical waste through incineration, electrolyte components decomposition in Li-ion batteries, consumer packaged good ozonolysis and many others. Current methodologies mostly rely on heuristic approaches rooted in a knowledge base of rules or cheminformatics.

In this webinar, we will present Schrödinger's enhanced Nanoreactor, extending the base tool developed by Grimme and co-workers [1]. Schrödinger Nanoreactor is a transformative digital solution for predicting chemical degradants of small molecules and sorting them directly from quantum mechanics and without any prior knowledge.

Webinar highlights

- Overview of the Nanoreactor technology which integrates automated potential energy surface exploration through semiempirical metadynamics, landscape refinement, and density functional theory-based sorting
- Demonstration of the user-friendly interface for identifying all possible degradation products, visualizing results, and classifying results based on thermodynamic principles - all from the computing power of a basic laptop
- Examples of how the technology can be applied to address challenges in pharmaceutical drug development, chemicals incineration, battery development, consumer packaged goods and more

1.Exploration of Chemical Compound, Conformer, and Reaction Space with Meta-Dynamics Simulations Based on Tight-Binding Quantum Chemical Calculations, Stefan Grimme, J. Chem. Theory Comput. 2019, 15, 5, 2847–2862

6 月 7 日(金)11:00-12:00

Materials Science Suite に含まれる
有機 EL 材料開発のためのプログラム紹介

シニア サイエンティスト　大塚　勇起

Materials Science Suite(MSS)には、有機 EL 材料の開発のために必要なプロパティ（励起エネルギー、酸化・還元ポテンシャル、再配置エネルギーや移動度等）を量子計算や機械学習により予測できるプログラムが含まれています。また、分子動力学（MD）計算を使用し、薄膜等の構造を再現・予測することも可能です。これらの機能を組み合わせることによって、スクリーニングや解析を行い、有機 EL 材料開発を効率化させることが可能です。本発表では、有機 EL 材料開発に関係する主なプログラムと共に、この１年でリリースされた新機能も含めて紹介します。