データ駆動型材料創製のための実在系計算化学とハイエントロピー材料への応用

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Real-system Computational Chemistry for Data-driven Materials Development and Its Applications to Multi-elemental High Entropy Materials (*Research Initiative for Supra Materials, Shinshu University*) ○Michihisa Koyama

The challenges in applying materials informatics to functional materials are to predict not only functionality but also stability, and to realize activity prediction that incorporates the heterogeneity of the active site structure of the real system. The author has clarified the origin of the properties that differ from those of the bulk by first-principles calculations of real systems that incorporate the real system structure without simplification by using a supercomputer. In addition, about 10,000 data points have been accumulated using nano-alloy structural models. In order not only to discover active new materials but also to create materials useful to society, it is important to construct a digital twin corresponding to physical space (physical space) in virtual space (cyberspace) to explore and evaluate materials at a throughput that surpasses that of experimental science. The author will present the details of ongoing efforts and future prospects, based on concrete examples in the multi-elemental materials.
Keywords : Computational Chemistry; Multi-element material; Real-system; Digital Screening

マテリアルズ・インフォマティクスを機能材料に適用する際の課題は、機能のみならず安定性を考慮した予測すること、実在系の活性点構造の不均一性を取り込んだ活性予測を実現することである 1)。著者は、スーパーコンピュータを用いることで実在系構造を簡略化せずに取り込んだ実在系第一原理計算によりバルクと異なる特性の起源を明らかにしてきた 2-13)。さらに、ナノ合金構造モデルを用いたデータを約 10,000 点蓄積してきた。

単に活性な新物質を発見するのみならず、社会に役立つ材料を創製するために、物理空間（フィジカルスペース）に対応したデジタルツインを仮想空間（サイバースペース）に構築し、実験科学を凌駕するスループットでの材料の探索、評価を実現することが重要である 14)。著者らがこれまでに取り組んできた多元素材料を具体例とした取り組みの詳細と今後の展望について紹介する。

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