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SPECIAL TOPIC — Stephen J. Pennycook: A research life in atomic-resolution STEM and EELS

A large language model-powered literature review for high-angle annular dark field imaging

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High-angle annular dark field (HAADF) imaging in scanning transmission electron microscopy (STEM) has become an indispensable tool in materials science due to its ability to offer sub-Å resolution and provide chemical information through Z-contrast. This study leverages large language models (LLMs) to conduct a comprehensive bibliometric analysis of a large amount of HAADF-related literature (more than 41000 papers). By using LLMs, specifically ChatGPT, we were able to extract detailed information on applications, sample preparation methods, instruments used, and study conclusions. The findings highlight the capability of LLMs to provide a new perspective into HAADF imaging, underscoring its increasingly important role in materials science. Moreover, the rich information extracted from these publications can be harnessed to develop AI models that enhance the automation and intelligence of electron microscopes.

Keywords: large language models, high-angle annular dark field imaging, deep learning

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1. Introduction

In scanning transmission electron microscopy (STEM), high-angle annular dark field (HAADF) imaging is probably the most popular microscopy technique.[1] HAADF images are formed by collecting electrons scattered at high angles while scanning a finely focused electron probe across a thin specimen. It offers sub-Å resolution, particularly with modern aberration-corrected microscopes.[2] It provides chemical information about the specimen, as the signal is dominated by thermal diffuse scattering that correlates strongly with the atomic number (Z) of the elements, known as Z-contrast.[3,4] Pennycook *et al.*[5] showed that the HAADF images are directly interpretable and do not have contrast reversal issues even in relatively thick crystalline samples, thanks to the incoherent nature of such scattering events. These characteristics have made HAADF imaging an indispensable tool in materials research, especially with the development and spread of aberration-corrected STEM instruments. The impact of HAADF imaging on materials science is evident from many excellent review papers and book chapters.[6–10] These works often focus on documenting technological advances or summarizing the applications of HAADF imaging in specific areas of materials science, such as catalysts[11,12] and electronic devices.[13,14]

The popularity of HAADF imaging has also led to the accumulation of a large body of literature that utilizes HAADF imaging, making it nearly impossible to conduct an exhaustive review. Large-scale literature analysis can be useful as it can provide an overarching trend of a research field, helping to identify gaps and provide researchers with a new perspective on research direction. An example is a recent work by Martín *et al.*[15] where they surveyed a few thousand of catalyst-research papers, and showed that catalyst deactivation is an area that did not get enough attention. However, they still used a conventional method to collect and analyze bibliometric data, which relies on the selection of carefully chosen search terms relevant to the subject, followed by a quantitative analysis of word frequencies within abstracts and titles. This type of method, with available tools like VOSviewer,[16] Bibliometrix[17] and Citespace,[18] still heavily depends on researchers' experience to pick the right search words to get the optimum results. While some mitigation solutions like standardized keywords exist (e.g., Medical Subject Headings (MeSH) by the National Institute of Health (NIH)), it is yet available in all fields. Another drawback of this conventional method is that many mainstream databases (e.g., Web of Science or PubMed) only offer free access to research papers' titles and abstracts, while possible search hits in other part of the paper can be overlooked. Finally, the conventional analysis based on word frequency lacks contextualization, often resulting in discrepancies between the intended meaning of a word and its appearance in the search results.

Recent advances in large language models (LLMs), exemplified by ChatGPT, have drawn significant attention due to their language comprehension and text generation capabilities.[19–23] The application of LLMs in large-scale bib-

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liometric analysis can be powerful. For instance, Yaghi and colleagues[24,25] used ChatGPT to collect information from a vast body of research literature about metal–organic frameworks (MOFs), and then developed a chatbot to give highly accurate feedback at fielding inquiries regarding the synthesis protocols of MOFs. Dagdelen *et al.*[26] also demonstrated that LLMs can accurately link dopants-matrix, cataloging MOFs and generating summary paragraphs of the materials from records of scientific papers. Polak *et al.*[27] demonstrated that ChatGPT can achieve close to 90% precision in extracting useful information from papers with the proper prompt engineering without the need to fine-tune the models themselves. Suvarna *et al*.[28] utilized LLMs to conduct a comprehensive literature review and analysis of single-atom heterogeneous catalysts (SACs).[28] These examples showcased the capabilities of LLMs for large-scale quantitative bibliometric analyses.

In this work, we utilized the LLMs to do a large-scale bibliometric data analysis for papers that contain HAADF imaging, which has rarely been done before. As an example of the application, we categorized those studies according to their research subjects, giving a more quantitative, and broader perspective on the impact of HAADF imaging on materials science. We will show that LLMs can also extract experiment-related parameters, such as sample preparation details, imaging conditions, etc., which might be useful for researchers studying similar materials. Finally, such bibliometric analysis can lead to a HAADF image database, which in turn can help train machine learning models for smart microscopy with the ability of automated image analysis.

2. Methods

2.1. Initial literature collection

We searched for research articles published from 1994 to May 2024 containing the word "HAADF" and "Z-contrast" on ScienceDirect. This search encompassed the entire article, not just the title and abstract. We obtained 41422 search results, which were exported and merged into a CSV file as the source data (supporting code 1 and supporting file 1).

2.2. Prompt engineering for text mining

The obtained data was entered into ChatGPT-3.5 along with a designed prompt (Fig. S1), which categorized the returned information under our defined headings. The results were then stored as a dictionary and logged into a CSV file for further statistical analysis.

2.3. Evaluation

The documents used for validation (682 in total, summarized in supporting file 2) were individually downloaded from selected high-impact journals (not necessarily from ScienceDirect). The reliability of GPT was evaluated by comparing the conclusions to those of research students, quantified by the F1 score. The confusion matrix for binary classification tasks is structured as follows: (a) true positives (TP): instances correctly predicted as positive; (b) true negatives (TN): instances correctly predicted as negative; (c) false positives (FP): instances incorrectly predicted as positive, also known as type I errors; (d) false negatives (FN): instances incorrectly predicted as negative, also known as type II errors. Precision (P) is defined as the ratio of TP to the total predicted positives: $P = \mathrm{TP}/(\mathrm{TP}+\mathrm{FP})$. Recall ($R$), or sensitivity, measures the ratio of TP to the actual positives: $R = \mathrm{TP}/(\mathrm{TP}+\mathrm{FN})$. The F1 score combines these two metrics into a single measure: $\mathrm{F1} = 2\times(P\times R)/(P+R)$.

2.4. Statistic analysis

Using the previously collected sample information and the 2024 Materials Research Society (MRS) Spring Meeting & Exhibit[29] as a categorization reference, we classified the materials based on their common applications into categories such as Electronics, Optics and Photonics, Energy and Environment, Quantum Physics, and Biomedical and Soft Materials. Each of these categories encompasses various subcategories. Additionally, we classified the materials according to their chemical compositions into categories such as Others, Soft Material, Thin Films, 2D Material, Oxides, Metal, Nanomaterial/Nano Particle, Polymer, and Ceramics. This classification allowed us to examine the distribution of applications of HAADF imaging from the perspective of the materials' chemical properties.

3. Results and discussion

We first conducted an initial literature survey using a conventional keyword search in the ScienceDirect database, chosen for its ability to search the entire content of articles, not just titles and abstracts. From this search, we collected information from documents including authors, article titles, abstracts, and more (supplementary file 1). This process yielded a sample set of 41422 documents.

For the next step of text mining, we designed a set of prompts to enable LLMs, specifically ChatGPT-3.5, to extract the desired information from this extensive dataset. We crafted a prompt to extract relevant parts from the abstracts of the documents in the dataset, saving these extracts in a new document. We fed the abstracts of the articles, along with the prompt, into ChatGPT-3.5. The AI returned information categorized under the headings: Sample Used, Instrument Used, General Analysis, and Conclusion. "Sample Used" refers to the samples characterized using HAADF-STEM in the document. "Instrument Used" denotes the model or type of STEM used in the study. "General Analysis" provides a one-sentence summary of the study's focus. "Conclusion" outlines the findings

of the document. Through prompt engineering, we enabled ChatGPT-3.5 to return a dictionary with the titles as keys and the relevant information as values, which we then recorded into a new CSV file.

As the detailed applications of publications involving HAADF imaging are classified by ChatGPT-3.5, the primary concern is the reliability of these results. To verify the accuracy of the information extracted by ChatGPT-3.5, we manually downloaded 682 documents from various sources (not just ScienceDirect) and compared the information described in these articles with the information extracted by ChatGPT-3.5. The results are summarized in Tables S1 and S2. For the application of materials, the accuracy was 0.8931, and the F1 score was 0.9315. For the classification of material properties, the accuracy reached 0.9531, and the F1 score was 0.9742. These results demonstrate ChatGPT-3.5's high accuracy in overall classification and text extraction tasks.

After confirming the credibility of ChatGPT-3.5's analysis results, we conducted a statistical analysis of its application classification. We aligned our classification with the topical clusters of the 2024 MRS Spring Meeting & Exhibit.[29] The results are shown in Fig. 1. Since 1994, the largest sector of literature involving HAADF imaging has been Energy and Environment, accounting for 67%, followed by Electronics, Optics, and Photonics at 14%, with Biomedical holding a small share of 5%. This trend indicates that over the past two decades, the rapidly developing field of Energy and Environment has led to a great demand for HAADF imaging techniques, leading to a significant increase in relevant literature in this area.

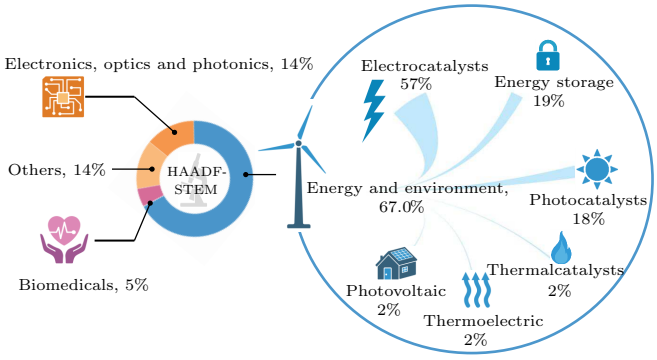


Fig. 1. The involvement of HAADF imaging in different fields (left) and more detailed sub-fields (right) within the Energy and Environment sector, derived from the large language models analysis of literature data obtained from ScienceDirect.

To further analyze the specific share distribution within the field of Energy and Environment, we referenced the symposium sessions of the 2024 MRS Spring Meeting & Exhibit,[29] summarizing them into six sub-fields: electrocatalysts, photocatalysts, thermal catalysts, photovoltaics, thermoelectrics, and energy storage (the right part of Fig. 1). The subdivisions for Electronics, Optics, and Photonics were analyzed similarly in a later section. The results show that electrocatalysts accounted for the largest proportion, more than half (57%), reflecting the intense research focus in recent years. Energy storage and photocatalysis followed with similar shares of 19% and 18%, respectively. The remaining subfields — photovoltaics, thermoelectrics, and thermal catalysts — each had a relatively small share of 2%.

We then selected two sectors and conducted a year-by-year analysis. Figure 2(a) illustrates that in the field of Energy and Environment, the number of papers involving HAADF imaging has increased annually, particularly in the last five years. This significant growth demonstrated the increasing importance of HAADF imaging. Additionally, it is evident that electrocatalysis consistently has the highest percentage in Energy and Environment. A similar growth pattern is observed in the field of Electronics, Optics, and Photonics. The number of publications utilizing HAADF has steadily increased, doubling over the past five years. Overall, these results demonstrate the rising number of publications employing HAADF across various fields.

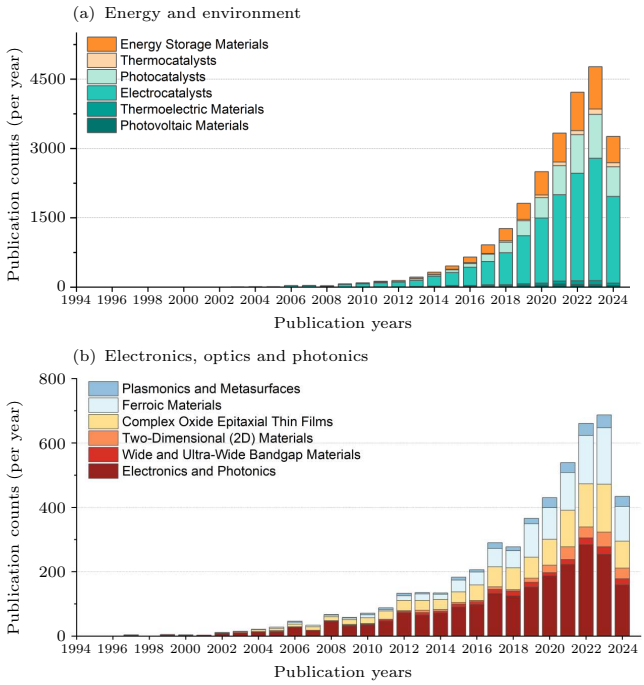


Fig. 2. Year-over-year growth trends of publications using HAADF on (a) Energy and Environment, and (b) Electronics, Optics and Photonics (publications collected from Elsevier only).

We want to visualize how important HAADF imaging has been to a particular research field. To achieve that, we chose Electrocatalysts and Complex Oxide Epitaxial Thin Films, both of which account for a significant proportion of the total number of publications in their respective fields, as representative research objects. We indexed all the literature published in the past 30 years from the ScienceDirect database and calculated the proportion of literature that involved HAADF in these two categories.

The results for Electrocatalysts, shown in Fig. 3(a), indicate that electrocatalysis research has been growing rapidly in the past decade. The proportion of HAADF used in electrocatalysis papers has steadily increased each year, reaching nearly 60% in the most recent year. This growing proportion suggests that while the field of electrocatalysis is developing independently, HAADF is becoming increasingly important and indispensable as a characterization technique, as reflected by its rising usage in the literature.

As shown in Fig 3(b), the number of yearly production of new publications on Complex Oxide Epitaxial Thin Films has remained relatively stable over the past 30 years, indicating consistent development in the field. However, the proportion of HAADF usage has increased steadily, rising from 10% to over 58% in the past ten years — nearly a six-fold increase. This trend once again highlights the growing influence of HAADF in various fields of materials science today.

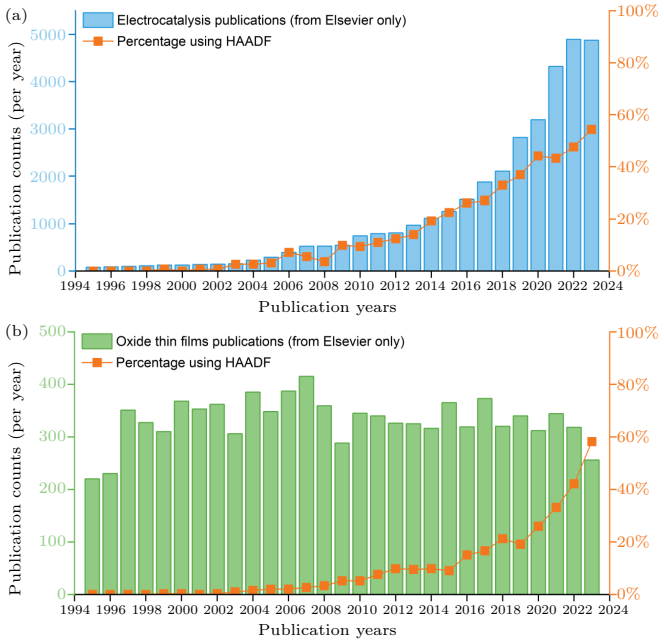


Fig. 3. The annual number of publications and the number of publications that HAADF imaging in (a) electrocatalysis and (b) oxide thin films research (publications collected from ScienceDirect only).

In addition to quantifying the impact of the HAADF technique through bibliometrics, the LLMs can also extract experimental details, which could potentially be useful for guiding subsequent experiments on similar materials. To demonstrate this capability, we selected three important parameters: the accelerating voltage of the microscope, the type of aberration corrector, and the method used for sample preparation. For our analysis, we needed the entire paper including supplementary information. Hence we used the previously mentioned 682 papers. If the literature did not elaborate on the experimental details, the specific parameters were categorized as "N.A." (not available).

The statistical results for the electron voltage are shown in Fig. 4(a). The mainstream accelerating voltages are concentrated at 200 kV (28%) and 300 kV (20%), with a smaller portion of the literature adopting accelerating voltages of 120 kV and below (9% in total). Regarding the choice of the corrector, more than half of the literature (61%) did not employ a corrector, while the rest were split between probe correctors and double correctors, with 17% and 12%, respectively. Additionally, the usage of correctors changing with time is also shown in Fig. S3. However, we noticed that in many papers, such experimental details are unfortunately not provided. In terms of sample preparation, the most widely used method is FIB/Lamellae (17%), followed by polishing + ion milling (11%). Other methods include electropolishing (7%), powder samples (5%), and ultramicrotomy (2%). It is clear that the LLMs can effectively summarize statistical results, providing valuable insights for researchers in the field.

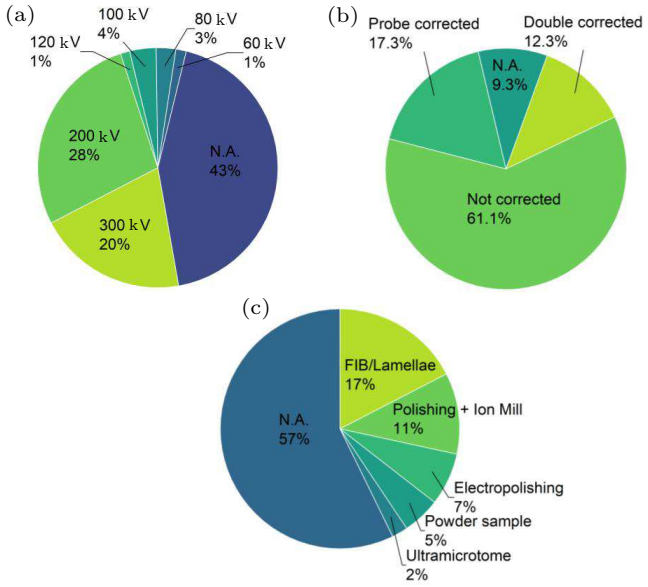


Fig. 4. Distribution of various HAADF parameters of selected 682 publications from selected high-impact journals. (a) Accelerating voltage. (b) Correction methods. (c) Sample preparation techniques.

Another potential application of an LLMs-powered literature survey is to create a database for HAADF images, as LLMs can link images with rich contextual information. As electron microscopes evolve to become increasingly intelligent and automated, the demand for training datasets for supervised learning intensifies.[30,31] Traditional methods of constructing image datasets for training can be broadly categorized into two approaches: (i) manual labeling of experimental data: while accurate, this method is inherently time-consuming and labor-intensive;[32,33] (ii) virtual datasets: these datasets, generated through physical simulations[34–38] or generative adversarial networks (GANs),[39–41] offer an alternative by eliminating manual labeling. However, they often struggle with generalization across diverse image types and domains.[42] LLMs can facilitate the extraction of electron microscopy images from textual sources. By amalgamating textual information such as sample descriptions and electron mi-

croscope details with the corresponding images, we can construct a multimodal database. This database would enhance automated methods for electron microscopy, as schematically illustrated in Fig. 5. This approach leverages the comprehensive understanding capabilities of LLMs to link images with detailed contextual information, thus providing a robust and versatile training resource for developing intelligent and automated electron microscopy techniques.

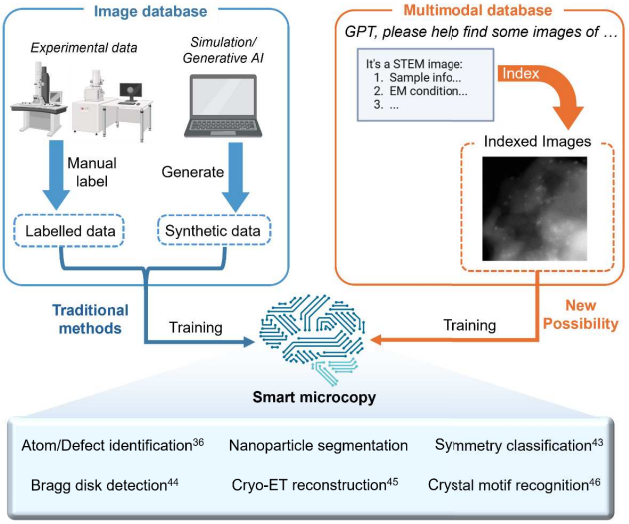


Fig. 5. A schematic illustration in smart microscopy through the use of image and multimodal databases.[36,43–46]

Our recent work[47] demonstrates the feasibility of training smart microscopy systems by indexing images from multimodal databases. As a simple example, we conducted a nanoparticle segmentation task. Firstly, we selected 20 real HAADF-STEM experimental images of our homemade PtSn@Al_2O_3 catalyst. Similarly, we retrieved 20 images extracted from the literature[48–56] using "PtSn@Al_2O_3" as the keyword from the built multimodal database. We used these two sets of images as training sets to train our segmentation network.[47] Detailed data processing and training methods are illustrated in Fig. S2, and the test results are shown in Figs. 6(a) and 6(b), respectively. The training results of the indexed images (Fig. 6(a)) were found to be comparable to the results from the real data (Fig. 6(b)), with most particles recognized and marked in red. The loss curve (Fig. 6(c)) indicates that both sets of images maintain a similar convergence rate. For Mean Intersection over Union (MIoU) shown in Fig. 6(d), which is a crucial evaluation metric for segmentation networks, the results from the indexed data are nearly equivalent to those from real experimental data, with only a negligible difference. Therefore, this verifies that extracting images from a multimodal database for the smart microscopy training dataset is feasible, and its training performance is almost indistinguishable from that of real data.

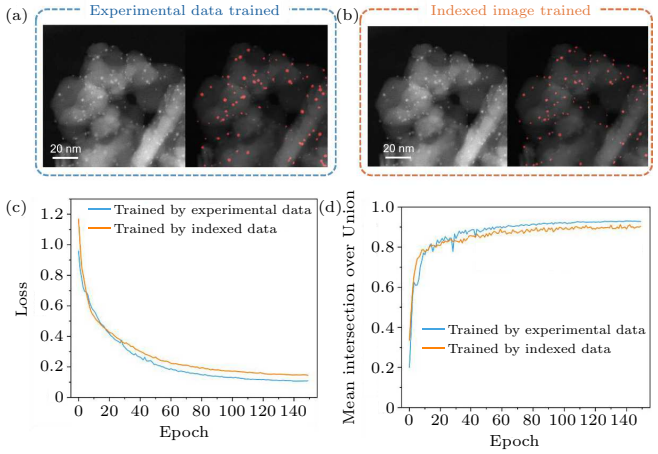


Fig. 6. Demo of using the constructed multimodal database to train nanoparticle segmentation network. (a) Segmentation result using the model trained by real data. (b) Segmentation result using the model trained by the multimodal database. (c) Loss curves of the two training methods. (d) Performance evaluation on MIoU of the two training methods.

4. Conclusion

A literature survey is an important part of our scientific endeavors. In this work, we carried out a large language model powered literature survey to cover a large number of published papers for the past 30 years that have involved HAADF imaging. The LLMs were able to understand the context of the papers, thus providing a more accurate analysis of the literature data. Through this analysis, we demonstrated the increasing importance of HAADF imaging in materials research. Perhaps more importantly, LLMs can extract useful information from the papers, such as experimental details that could potentially guide follow-up research. We also showed that by linking the correct context to HAADF images published in the literature, we can create an image database that can help train AI models for automated data analysis. This was exemplified by our recent work on particle analysis from HAADF and other types of TEM images. In summary, we demonstrated that LLMs offer new perspectives on the vast amount of literature involving HAADF imaging, highlighting its growing significance in materials research. Additionally, we showed that there is a wealth of information in these publications that could potentially be used to train AI models for automatic data analysis, making electron microscopes smarter.

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References

[1] Pennycook S J and Nellist P D 2011 *Scanning transmission electron microscopy: imaging and analysis* (Springer Science & Business Media)

[2] Nellist P D, Chisholm M F, Dellby N, Krivanek O L, Murfitt M F, Szilagyi Z S, Lupini A R, Borisevich A, Sides W H Jr and Pennycook S J 2004 *Science* **305** 1741

[3] Pennycook S J 1989 *Ultramicroscopy* **30** 58

[4] Pennycook S J and Boatner L A 1988 *Nature* **336** 565

[5] Pennycook S J and Jesson D E 1990 *Phys. Rev. Lett.* **64** 938

[6] Varela M, Lupini A R, van Benthem K, Borisevich A Y, Chisholm M F, Shibata N, Abe E and Pennycook S J 2005 *Annu. Rev. Mater. Res.* **35** 539

[7] Pennycook S J, Li C J, Li M S, Tang C H, Okunishi E, Varela M, Kim Y M and Jang J H 2018 *J. Anal. Sci. Technol.* **11** 14

[8] Pennycook S J 2012 *Ultramicroscopy* **123** 28

[9] Sousa A A and Leapman R D 2012 *Ultramicroscopy* **123** 38

[10] Kalinin S V, Ophus C, Voyles P M, Erni R, Kepaptsoglou D, Grillo V, Lupini A R, Oxley M P, Schwenker E, Chan M K Y, Etheridge J, Li X, Han G G D, Ziatdinov M, Shibata N and Pennycook S J 2022 *Nat. Rev. Methods Primers* **2** 11

[11] Wang Z L 2003 *Adv. Mater.* **15** 1497

[12] Zhang T J, Walsh A G, Yu J H and Zhang P 2021 *Chem. Soc. Rev.* **50** 569

[13] Wu H J, Zhang Y, Ning S C, Zhao L D and Pennycook S J 2019 *Mater. Horiz.* **6** 1548

[14] Gáquez J, Sánchez-Santolino G, Biškup N, Roldán M A, Cabero M, Pennycook S J and Varela M 2017 *Mater. Sci. Semicond. Process.* **65** 49

[15] Martín A J, Mitchell S, Mondelli C, Jaydev S and Pérez-Ramírez J 2022 *Nat. Catal.* **5** 854

[16] Van Eck N and Waltman L 2010 *Scientometrics* **84** 523

[17] Aria M and Cuccurullo C 2017 *J. Informetr.* **11** 959

[18] Chen C, Hu Z, Liu S and Tseng H 2012 *Expert Opin. Biol. Ther.* **12** 593

[19] Zhang Q, Ding K, Lyv T, Wang X, Yin Q, Zhang Y, Yu J, Wang Y, Li X and Xiang Z 2024 arXiv: 2401.14656

[20] Thirunavukarasu A J, Ting D S J, Elangovan K, Gutierrez L, Tan T F and Ting D S W 2023 *Nat. Med.* **29** 1930

[21] Choi J and Lee B 2024 *Commun. Mater.* **5** 13

[22] Zhao Z, Ma D, Chen L, Sun L, Li Z, Xu H, Zhu Z, Zhu S, Fan S and Shen G 2024 2024 arXiv: 2401.14818

[23] Rubungo A N, Arnold C, Rand B P and Dieng A B 2023arXiv:2310.14029

[24] Zheng Z, Zhang O, Borgs C, Chayes J T and Yaghi O M 2023 *J. Am. Chem. Soc.* **145** 18048

[25] Zheng Z, Rong Z, Rampal N, Borgs C, Chayes J T and Yaghi O M 2023 *Angew. Chem. Int. Ed. Eng.* **62** e202311983

[26] Dagdelen J, Dunn A, Lee S, Walker N, Rosen A S, Ceder G, Persson K A and Jain A 2024 *Nat. Commun.* **15** 1418

[27] Polak M P and Morgan D 2024 *Nat. Commun.* **15** 1569

[28] Suvarna M, Vaucher A C, Mitchell S, Laino T and Perez-Ramirez J 2023 *Nat. Commun.* **14** 7964

[29] https://www.mrs.org/meetings-events/spring-meetings-exhibits/2024-mrs-spring-meeting

[30] Kalinin S V, Mukherjee D, Roccapriore K, Blaiszik B J, Ghosh A, Ziatdinov M A, Al-Najjar A, Doty C, Akers S, Rao N S, Agar J C and Spurgeon S R 2023 *npj Comput. Mater.* **9** 227

[31] Spurgeon S R, Ophus C, Jones L, Petford-Long A, Kalinin S V, Olszta M J, Dunin-Borkowski R E, Salmon N, Hattar K, Yang W C D, Sharma R, Du Y, Chiaramonti A, Zheng H, Buck E C, Kovarik L, Penn R L, Li D, Zhang X, Murayama M and Taheri M L 2021 *Nat. Mater.* **20** 274

[32] Sun Z, Shi J, Wang J, Jiang M, Wang Z, Bai X and Wang X 2022 *Nanoscale* **14** 10761

[33] Liu S, Zhang F, Lin R and Liu W 2022 *Chem. Res. Chin. Univ.* **38** 1263

[34] Treder K P, Huang C, Bell C G, Slater T J A, Schuster M E, Özkaya D, Kim J S and Kirkland A I 2023 *npj Comput. Mater.* **9** 18

[35] Lin R, Zhang R, Wang C, Yang X Q and Xin H L 2021 *Sci. Rep.* **11** 5386

[36] Chu T, Zhou L, Zhang B and Xuan F Z 2023 *Nano Res.* **17** 2971

[37] Faraz K, Grenier T, Ducottet C and Epicier T 2022 *Sci. Rep.* **12** 2484

[38] Zhu D, Wang C, Zou P, Zhang R, Wang S, Song B, Yang X, Low K B and Xin H L 2023 *Nano Lett.* **23** 8272

[39] Khan A, Lee C H, Huang P Y and Clark B K 2023 *npj Comput. Mater.* **9** 85

[40] Bals J and Epple M 2023 *Adv. Intell. Syst.* **5** 2300004

[41] Cheng X, Xie C, Liu Y, Bai R, Xiao N, Ren Y, Zhang X, Ma H and Jiang C 2024 *Chin. Phys. B* **33** 030703

[42] Jacobs R 2022 *Comput. Mater. Sci.* **211** 111527

[43] Ziletti A, Kumar D, Scheffler M and Ghiringhelli L M 2018 *Nat. Commun.* **9** 2775

[44] Munshi J, Rakowski A, Savitzky B H, Zeltmann S E, Ciston J, Henderson M, Cholia S, Minor A M, Chan M K Y and Ophus C 2022 *npj Comput. Mater.* **8** 254

[45] Powell B M and Davis J H 2024 *Nat Methods* **21** 1525

[46] Akers S, Kautz E, Trevino-Gavito A, Olszta M, Matthews B E, Wang L, Du Y and Spurgeon S R 2021 *npj Comput. Mater.* **7** 187

[47] Yuan W, Yao B, Tan S, You F and He Q 2024 arXiv: 2407.19544

[48] Jang E J, Lee J, Jeong H Y and Kwak J H 2019 *Appl. Catal. A: Gen.* **572** 1

[49] Wang Z, Chen Y, Mao S, Wu K, Zhang K, Li Q and Wang Y 2020 *Adv. Sustain. Syst.* **4** 2000092

[50] Zhang J, Deng Y, Cai X, Chen Y, Peng M, Jia Z, Jiang Z, Ren P, Yao S, Xie J, Xiao D, Wen X, Wang N, Liu H and Ma D 2019 *ACS Catal.* **9** 5998

[51] Xu Z, Yue Y, Bao X, Xie Z and Zhu H 2020 *ACS Catal.* **10** 818

[52] Wan H, Qian L, Gong N, Hou H, Dou X, Zheng L, Zhang L and Liu L 2023 *ACS Catal.* **13** 7383

[53] Singh J, Nelson R C, Vicente B C, Scott S L and van Bokhoven J A 2010 *Physical Chemistry Chemical Physics* **12** 5668

[54] Yang F, Zhang J, Chen J, Wang G, Yu T, Li Q, Shi Z, Sun Q, Zhuo R and Wang R 2024 *Nano Res.* **17** 5884

[55] Xu C, Tan S, Tang Y, Xi S, Yao B, Wade A, Zhao B, Lu S, Du Y, Tian M, He C, Ma L, Fu X, Shi J, Lu J, Howe A G R, Dai S, Luo G and He Q 2024 *Appl. Catal. B* **341** 123285

[56] Xie J, Jiang H, Qian Y, Wang H, An N, Chen S, Dai Y and Guo S 2021 *Advanced Materials Interfaces* **8** 2101325