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Highlights

Multimodal Literature Mining for Autonomous Hydrogen Storage Materials Discovery

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The rapid expansion of artificial intelligence (AI) in chemistry and materials science has greatly accelerated data analysis and property prediction. These advances rely heavily on well-curated experimental databases, for which the scientific literature remains the richest source. However, much of this information is not written explicitly in the text, but encoded in figures such as pressure-composition-temperature (PCT) curves and temperature-programmed desorption (TPD) profiles. Conventional literature-mining workflows can locate these figures, but often struggle to interpret the relationships between material composition, experimental conditions and measured performance. Converting this figure-embedded knowledge into machine-readable form therefore remains a central challenge for autonomous materials discovery.

In a recent study [1], Zhang et al. introduced the Descriptive Interpretation of Visual Expression (DIVE) (Figure 1), a multi-agent workflow designed to systematically convert figure-embedded experimental information into machine-readable scientific knowledge. Applied to over 4000 publications on hydrogen storage materials, DIVE was used to construct the Digital Hydrogen Platform (DigHyd), comprising more than 30,000 experimentally derived entries spanning over five decades of hydrogen-storage research.

Rather than directly feeding figures into multimodal LLMs for extraction, DIVE introduces a conceptually elegant intermediate step: transforming visual information into descriptive textual representations before structured extraction. This "visual-to-language" strategy substantially improves extraction robustness and completeness, enabling performance gains of 10–15% over leading commercial models and up to 30% over open-source alternatives. Importantly, the work highlights a growing realization in AI-assisted chemistry: reliable scientific reasoning often depends not only on larger models, but also on carefully designed workflows that reshape how information is represented and processed.

The significance of this work extends beyond database construction. By integrating the DigHyd database with machine-learning verification models and LLM-based reasoning, the authors established an AI agent capable of proposing, evaluating, and iteratively refining candidate hydrogen storage materials under user-defined constraints. In one representative example, the system progressively optimized candidate compositions from $CaMgFe_2$ to $Mg_2Fe_{0.6}Co_{0.2}Mn_{0.2}$ through a multi-step reasoning and evaluation process. Such iterative refinement begins to resemble aspects of real scientific decision-making rather than simple data retrieval or static prediction.

This shift from conventional literature mining toward AI-assisted materials reasoning represents a key conceptual advance of DIVE and DigHyd. Rather than using AI only for property prediction, text extraction or virtual screening, the workflow moves toward a "literature-to-design" paradigm, in which experimental knowledge is extracted, organized and used to propose and refine candidate materials. In this sense, DIVE connects data extraction with materials design, rather than treating them as separate tasks.

Overall, DIVE and DigHyd demonstrate how multimodal AI can turn literature-embedded experimental knowledge into a practical route for materials design. By connecting scientific figures, structured databases, machine-learning models and design agents, this work moves beyond conventional data extraction and prediction toward a "literature-to-design" paradigm. Although challenges remain in figure interpretation, experimental

validation and extrapolation beyond known chemical spaces, it represents an important step toward autonomous scientific reasoning and closed-loop materials discovery.

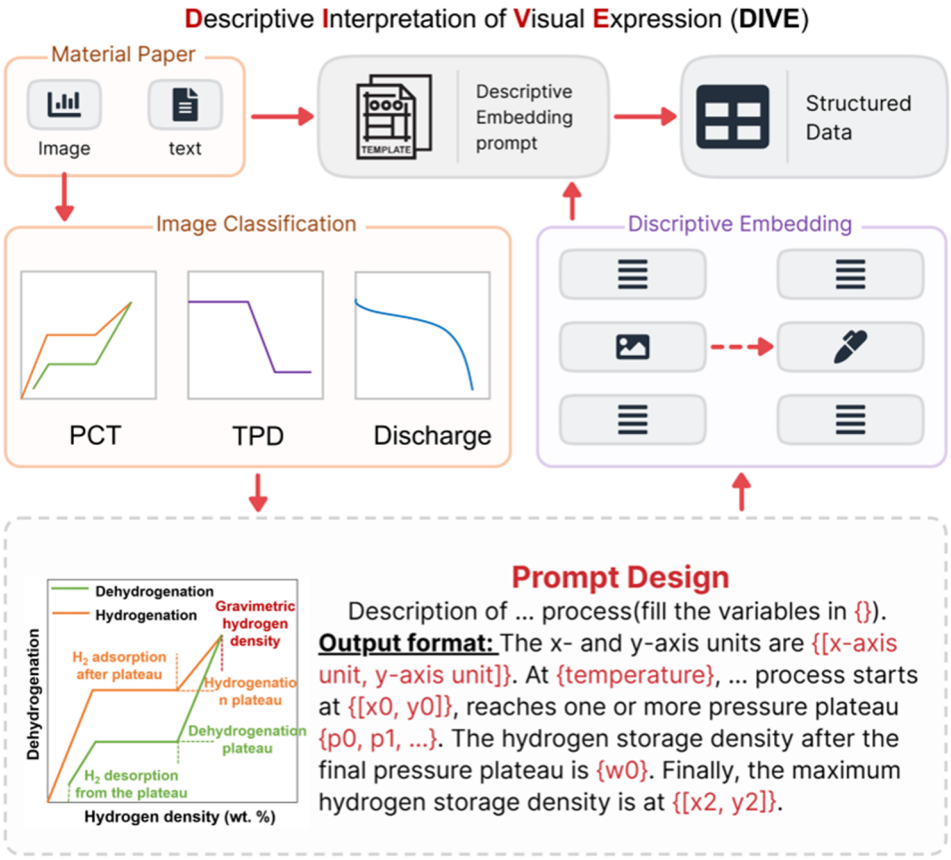

Figure 1. Overview of the DIVE workflow: key figure information is first converted into descriptive text prompts, then used for structured data extraction. PCT refers to pressure-composition-temperature curves, and TPD refers to temperature-programmed desorption curves. Adapted from Ref. [1].

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Conflicts of Interest

The author declares no conflict of interest.

Use of AI and AI-Assisted Technologies

During the preparation of this work, the author used ChatGPT (OpenAI) to improve the clarity, grammar, and readability of the manuscript. After using this tool, the author reviewed and edited the content as needed and take full responsibility for the content of the published article.

Reference

1. Zhang, D.; Jia, X.; Tran, H.B.; et al. “DIVE” into Hydrogen Storage Materials Discovery with AI Agents. *Chem. Sci.* **2026**, *17*, 3031–3042. https://doi.org/10.1039/d5sc09921h.