

Beyond Static Kinetics: The Burst Effect Reveals Dynamic Evolution in MgH_2 Dehydrogenation

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Abstract

Mg-based hydrides are promising solid-state hydrogen storage materials, but their practical application remains limited by sluggish dehydrogenation kinetics, particularly at the onset of hydrogen release. In conventional studies, the literature-reported apparent activation energy derived from Arrhenius analysis is widely used to evaluate dehydrogenation behavior. However, this parameter does not adequately capture the kinetic limitation controlling onset dehydrogenation, indicating that MgH_2 dehydrogenation cannot be fully understood within a static kinetic framework. In this work, layer-dependent theoretical barriers, dynamic kinetic reconstruction, and literature-scale statistical analysis were combined to compare the relationships of literature-reported apparent activation energy and initial dehydrogenation activation energy with onset dehydrogenation temperature in Mg-based systems. The results show that MgH_2 dehydrogenation follows a dynamically evolving barrier process characterized by the burst and plateau regions. Within this framework, the literature-reported apparent activation energy exhibits only a weak correlation with onset dehydrogenation temperature, whereas the initial dehydrogenation activation energy shows a much stronger positive correlation. These results indicate that onset dehydrogenation is more directly associated with the initial high-barrier stage than with the averaged kinetic behavior of the subsequent stable stage. This work moves beyond static kinetics and provides a clearer dynamic kinetic framework for understanding onset dehydrogenation in Mg-based hydrogen storage materials.

1. Introduction

Safe and efficient hydrogen storage is an essential prerequisite for the large-scale deployment of hydrogen energy [1-3]. Among solid-state hydrogen storage systems, Mg-based hydrides are widely regarded as promising candidates because of their high hydrogen capacity, low cost, and natural abundance [4]. However, the practical application of MgH_2 remains severely hindered by sluggish dehydrogenation kinetics, particularly during the onset stage of hydrogen release [5-7]. Considerable efforts have therefore been devoted to improving its dehydrogenation performance, among which catalytic modification has been recognized as one of the most effective strategies [8-12]. In the evaluation of catalytic performance, the apparent dehydrogenation activation energy derived from Arrhenius analysis is still commonly used as a key kinetic parameter [13,14]. However, this averaged parameter does not reliably describe onset dehydrogenation behavior. For example, catalysts such as TiV-MgO , Ti_2VAlC_2 MAX, $\text{CuSA/Ti}_3\text{C}_2\text{T}_x$, and $\text{Ni}_{0.034}\text{@TiO}_2$ can reduce the literature-reported apparent activation energy to 96.2, 78, 76.38, and 64.35 kJ/mol, respectively, whereas their onset dehydrogenation temperatures still remain as high as 202, 204, 241.73, and 200 °C [15-18]. These results indicate that the literature-reported apparent activation energy does not adequately capture the initial kinetic limitation governing onset dehydrogenation, suggesting that the dehydrogenation behavior of MgH_2 cannot be fully understood within a static averaged kinetic framework.

The origin of this inconsistency lies in the fact that MgH_2 dehydrogenation is not governed by a single static barrier. Instead, hydrogen release involves coupled processes such as bulk hydrogen migration, surface diffusion, and surface desorption, while the MgH_2 surface continuously evolves during reaction [19]. Accordingly, the kinetic barrier varies with reaction progress rather than remaining constant. Previous theoretical studies have shown that the barrier for first-layer hydrogen desorption is substantially higher than those for subsequent hydrogen release steps, whereas migration-related barriers remain comparatively low [20-22]. Consistently, dynamic kinetic reconstruction based on segmented analysis has shown that the dehydrogenation activation energy exhibits a clear decline-then-stabilization evolution with reaction progress [23,24]. Recent dynamic thermodynamic analysis further indicates that the reaction enthalpy response of Mg-based dehydrogenation is also dynamic, and its turning behavior is broadly consistent with the evolution of dynamic activation energy [25]. This progress-dependent decrease followed by barrier stabilization is referred to as the burst effect. This effect reflects the transition of MgH_2 dehydrogenation from an initially hindered stage to a more stabilized hydrogen release stage. Taken together, these findings indicate that MgH_2 dehydrogenation should be interpreted primarily as a dynamically evolving kinetic process, while the accompanying dynamic thermodynamic response provides complementary support for its stage-dependent nature. Under such a dynamic kinetic framework, the kinetic parameter governing onset dehydrogenation is unlikely to be the conventional activation energy reported in the literature, which is extracted from averaged reaction behavior, but is more plausibly associated with the initial high-barrier segment of the dehydrogenation process.

On this basis, this work combines layer-dependent theoretical barriers, dynamic kinetic reconstruction, and literature-scale statistical analysis to compare the conventional activation energy reported in the literature with the initial dehydrogenation activation energy in Mg-based systems. Their respective relationships with onset dehydrogenation temperature are then examined to identify the descriptor more closely related to the initial hydrogen release process. By moving beyond static kinetics, this work uses the burst effect as a physically grounded framework to reveal the dynamic evolution of dehydrogenation barriers in MgH_2 and to clarify its implications for onset behavior, kinetic evaluation, and catalytic regulation in Mg-based hydrogen storage materials.

2. Methods and Data Curation

The data used in this study consisted of three categories: layer-dependent theoretical barrier data, literature-reported isothermal dehydrogenation kinetic data, and literature-reported onset dehydrogenation temperatures paired with apparent activation energy values. First-layer and subsequent-layer hydrogen desorption barriers, together with hydrogen migration barriers, were obtained from previous density functional theory studies and used to characterize the barrier differences among distinct reaction steps during MgH_2 dehydrogenation. On this basis, published isothermal dehydrogenation curves were further analyzed to examine the evolution of dehydrogenation activation energy with reaction progress. For the macroscopic kinetic analysis, a dynamic reconstruction method

based on segmented analysis was applied to the isothermal dehydrogenation data. Following the analytical procedure previously established from the distributed activation energy model, kinetic parameters were reconstructed over successive reaction progress intervals to obtain dynamic activation energy curves along reaction progress. The initial dehydrogenation activation energy and the subsequent plateau-stage activation energy were then extracted from the reconstructed curves [23].

To evaluate the generality of these kinetic features in Mg-based systems, published dehydrogenation data were statistically compiled from the solid-state hydrogen storage database *Digital Hydrogen-S* [26-30]. Dynamic dehydrogenation activation energy curves were reconstructed for different systems, and their distribution characteristics were statistically analyzed [31]. In addition, literature-reported onset dehydrogenation temperatures and apparent activation energy values were collected and compared with the reconstructed initial dehydrogenation activation energy. The analysis focused on three aspects: the discrepancy between theoretically calculated activation energy and experimentally fitted apparent activation energy, the correlation between literature-reported apparent activation energy and onset dehydrogenation temperature, and the correlation between initial dehydrogenation activation energy and onset dehydrogenation temperature. The origin of the theoretical-experimental discrepancy was further interpreted by comparing the initial stage and the plateau stage of the dynamic activation energy curve. These comparisons were used to clarify the relationships between different kinetic parameters and initial dehydrogenation behavior.

3. Results and Discussion

MgH₂ dehydrogenation cannot be adequately described by a single constant activation energy. Instead, it should be understood as a barrier-evolution process that varies with reaction progress. During dehydrogenation, the MgH₂ surface evolves continuously, and neither the catalyst-contacting interface nor the local reaction environment remains unchanged (**Figure 1a**). Layer-dependent theoretical barriers show that the first-layer hydrogen desorption barrier is substantially higher than those for the second and third layers, whereas hydrogen migration barriers remain consistently lower than desorption barriers (**Figure 1b**) [20-22]. These results indicate that the initial stage of MgH₂ dehydrogenation is associated with a distinctly higher kinetic barrier. They also indicate that surface dehydrogenation, rather than bulk hydrogen migration, remains the rate-determining step throughout the dehydrogenation process. Consistently, the reconstructed activation energy curve obtained from dynamic kinetic analysis exhibits a clear decline-then-stabilization evolution with reaction progress (**Figure 1c**) [23,24]. On this basis, the initial stage characterized by a rapid barrier drop can be defined as the burst region, whereas the subsequent relatively stable stage can be defined as the plateau region. In this framework, the starting point of the curve corresponds to the initial dehydrogenation barrier and directly reflects the rate-controlling feature at the onset of reaction. The slope characterizes the rate of barrier release. The inflection point marks the transition from the rapid-drop stage to the stable stage. The plateau represents the apparent barrier level in the subsequent stable hydrogen release regime. Accordingly,

MgH₂ dehydrogenation is more appropriately represented by a dynamic activation energy curve than by a single averaged activation energy.

This dynamic barrier evolution is not an isolated phenomenon. A statistical analysis across pristine MgH₂, catalyst-modified systems, and alloyed systems shows that the reconstructed activation energy curves of different Mg-based systems all display a similar decline-then-stabilization trend (**Figure 2a**) [34-58]. This result indicates that the burst region and plateau region are not material-specific or condition-specific features, but rather common dynamic kinetic characteristics of Mg-based dehydrogenation. In addition, the reconstructed dynamic activation energy data exhibit an overall unimodal, Gaussian-like distribution (**Figure 2b**), which is consistent with the statistical characteristics expected from the distributed activation energy model [31]. Together, these results suggest that the initial high-barrier stage and the subsequent stabilized stage have clear physical and statistical foundations. This observation provides the foundation for comparing the relationships between different kinetic parameters and onset dehydrogenation behavior.

Within this dynamic barrier-evolution framework, the long-standing discrepancy between theoretically calculated activation energy and experimentally fitted apparent activation energy can be explained more clearly [32,33]. The statistical results show that the mean theoretical and experimental activation energy values compiled from the literature are 210.70 and 135.96 kJ mol⁻¹, respectively, with an average difference of 74.75 kJ mol⁻¹ (**Figure 3a**). After the dynamic dehydrogenation activation energy curve is further divided into the burst region and the plateau region, the mean initial dehydrogenation activation energy and plateau-stage activation energy are 195.94 and 129.47 kJ mol⁻¹, respectively, corresponding to a difference of 66.47 kJ mol⁻¹ (**Figure 3b**). The close agreement between these two differences indicates that the theoretical and experimental activation energy data should not be regarded as contradictory kinetic descriptions, but instead correspond to barrier information from different stages of the same dynamic dehydrogenation process. Theoretical calculations generally probe the initial high-barrier stage associated with first-layer hydrogen desorption. This stage corresponds to the front part of the burst region. By contrast, the conventionally fitted apparent activation energy mainly reflects the averaged kinetic behavior dominated by the plateau region. Therefore, the literature-reported apparent activation energy does not directly represent the kinetic limitation at the onset stage, but is closer to the averaged barrier level of the subsequent stabilized stage.

A further comparison between different kinetic parameters and onset dehydrogenation temperature shows that the literature-reported apparent activation energy is not suitable as a standalone descriptor of onset dehydrogenation behavior [53-65]. The literature-reported apparent activation energy exhibits only a weak correlation with onset dehydrogenation temperature, with $R^2 = 0.087$ (**Figure 3c**). In contrast, the initial dehydrogenation activation energy shows a much stronger positive correlation with onset dehydrogenation temperature, with $R^2 = 0.645$ (**Figure 3d**). These results indicate that onset dehydrogenation is not governed primarily by the averaged barrier represented by the plateau region, but is more directly associated with the initial high barrier represented by the starting point of the burst

region. Compared with the literature-reported apparent activation energy, the initial dehydrogenation activation energy therefore more accurately reflects the kinetic limitation during initial hydrogen release and provides a better explanation for the variation in onset dehydrogenation temperature among different Mg-based systems..

The comparison of dynamic dehydrogenation activation energy curves under different catalysts further supports this interpretation. The effect of different catalysts is not manifested as a simple uniform downward shift of the entire activation energy curve, but is reflected in changes in the starting point, slope, inflection point, and plateau of the curve (**Figure 3e-g**) [63-65]. This result indicates that catalytic regulation is strongly stage-selective, with different catalysts influencing different regions of the dynamic barrier profile rather than uniformly lowering the barrier throughout the process. Among these characteristic regions, the initial dehydrogenation activation energy associated with the curve starting point remains the descriptor most directly related to onset dehydrogenation behavior, whereas the plateau region mainly reflects the averaged kinetic behavior of the later stage. Therefore, kinetic analysis of onset dehydrogenation in Mg-based hydrogen storage materials should not rely solely on the literature-reported apparent activation energy, but should pay greater attention to the initial high-barrier feature represented by the starting point of the burst region and its direct relationship with initial hydrogen release behavior.

4. Conclusions

In conclusion, MgH_2 dehydrogenation cannot be adequately described by a single constant activation energy, but should instead be understood as a dynamically evolving barrier-governed process. Layer-dependent theoretical barriers and dynamic kinetic reconstruction reveal a transition from an initial high-barrier stage to a subsequent stabilized stage, corresponding to the burst and plateau regions, respectively. The initial high barrier associated with first-layer hydrogen desorption represents the major kinetic limitation at the onset of hydrogen release. Statistical analysis further shows that the literature-reported apparent activation energy correlates only weakly with onset dehydrogenation temperature, whereas the initial dehydrogenation activation energy shows a much stronger correlation. This result indicates that onset dehydrogenation is more directly associated with the starting point of the burst region than with the averaged barrier represented by the plateau region.

These findings suggest that kinetic evaluation and catalytic regulation of Mg-based hydrogen storage materials should move beyond a static averaged activation energy description. For material evaluation, greater attention should be paid to the relationship between initial dehydrogenation activation energy and onset dehydrogenation temperature. For catalytic regulation, different catalysts should be assessed according to their effects on distinct regions of the dynamic barrier curve, including the starting point, slope, inflection point, and plateau. Since the curve starting point is most closely related to onset hydrogen release, catalyst regulation should pay more attention to first-layer hydrogen desorption. More broadly, dynamic evidence from barrier evolution and thermodynamic response suggests that Mg-based dehydrogenation should be examined using dynamic descriptors rather than a single averaged

parameter. Overall, this work provides a stage-resolved dynamic kinetic perspective for linking microscopic barrier evolution with macroscopic onset dehydrogenation behavior and for interpreting onset behavior and catalyst effects in Mg-based hydrogen storage materials.

Declarations

CRedit author statement

Jianghao Cai: Writing - Original Draft, Methodology, Software, Visualization, Writing - Review & Editing. **Kang Ma:** Formal analysis, Visualization. **Yutong Jiang:** Formal analysis, Data Curation. **Mingzhe Li:** Writing - Review & Editing. **Tangxuan Gao:** Formal analysis, Data Curation. **Tongao Yao:** Methodology, Visualization. **Zhengyang Gao:** Writing - Review & Editing, Funding acquisition. **Weijie Yang:** Conceptualization, Writing - Review & Editing, Supervision, Funding acquisition.

Data availability

The datasets used and analyzed during the current study are available from the corresponding author upon reasonable request.

Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Declaration of generative AI and AI-assisted technologies in the writing process

During the preparation of this work, the authors used ChatGPT in order to improve language expression and check grammar. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the publication.

References

1. M. Allendorf, V. Stacila, J. Snider, et al. Challenges to developing materials for the transport and storage of hydrogen. *Nat. Chem.* 14 (2022) 1214-1223. <https://doi.org/10.1038/s41557-022-01056-2>.

2. T. Yao, Y. Yang, Y. Yan, et al. Knowledge-extractor: a self-evolving scientific framework for hydrogen energy research driven by AI agents. *AI Agent* 1 (2025) 7.
<https://dx.doi.org/10.20517/aiagent.2025.04>
3. Y. Yang, F. Su, Q. Fang, et al. Study on the mechanism of Ni and Pr doping to improve the hydrogen absorption and desorption properties of Mg₉₅Ni₂Pr₃ hydrogen storage alloy. *J. Energy Storage* 169 (2026) 122662. <https://doi.org/10.1016/j.est.2026.122662>.
4. Y. Zhu, M. Tuluhong, Y. Ji, et al. Thermo-hydrogen coupling characteristics of Mg-based hydrogen storage materials and thermal management. *Energy Storage Mater.* 83 (2025) 104720.
<https://doi.org/10.1016/j.ensm.2025.104720>.
5. W. Fu, Y. Li, X. Yang, et al. Toward intelligent design of solid-state hydrogen storage: trends, challenges, and machine learning insights. *ENG. Chem. Eng.* 20 (2026) 25.
<https://doi.org/10.1007/s11705-026-2649-3>.
6. P. Zhou, Q. Zhou, W. Liu, et al. Resolving the capacity-stability-cost trilemma in multi-principal-element hydrogen storage alloys through multi-objective optimization. *Adv. Sci.* 12(43) (2025) e13463. <https://doi.org/10.1002/adv.202513463>.
7. H. Yang, Z. Ding, Y. Li, et al. Recent advances in kinetic and thermodynamic regulation of magnesium hydride for hydrogen storage. *Rare Met.* 42(9) (2023) 2906-2927.
<https://doi.org/10.1007/s12598-023-02306-z>.
8. C. Wang, X. Hou, H. Liu, et al. Catalytic modifications to enhance the hydrogen storage behavior of Mg-based materials: Single-component, multi-component single-phase and multiphase interfacial composite catalytic. *J. Energy Chem.* 110 (2025) 393-426.
<https://doi.org/10.1016/j.jechem.2025.06.071>.
9. T. Yao, J. Huang, Y. Yan, et al. From large language models to AI agents in energy materials research: enabling discovery, design, and automation. *AI Agent* 1 (2025) 9.
<https://dx.doi.org/10.2517/aiagent.2025.03>
10. H. Jiang, Z. Ding, Y. Li, et al. Hierarchical interface engineering for advanced magnesium-based hydrogen storage: synergistic effects of structural design and compositional modification. *Chem. Sci.* 16 (2025) 7610. <https://doi.org/10.1039/D5SC01169H>.
11. X. Lu, S. Luo, J. Li, et al. FIND: a forward-inverse navigation and discovery platform for hydrogen storage alloys powered by data-driven machine learning. *J. Mater. Inf.* 5 (2025) 48.
<https://dx.doi.org/10.20517/jmi.2025.5>.
12. X. Tang, J. Cai, T. Yao, et al. Revealing the role of grain boundaries in magnesium-based hydrogen storage: insights into adsorption and dissociation. *J. Mater. Chem. A* 13 (2025) 38252.
<https://doi.org/10.1039/D5TA04858C>.
13. M. Fanfoni, M. Tomellini. The Johnson-Mehl-Avrami-Kohnogorov model: A brief review. *IL Nuovo Cimento* 20 (1998) 1171-1182. <https://doi.org/10.1007/BF03185527>.
14. T. Huang, C. Zhou. Surface diffusion-controlled Jonhson-Mehl-Avrami- Kolmogorov model for hydrogenation of Mg-based alloys. *J. Phys. Chem. C* 127 (2023), 13900-13910.

<https://doi.org/10.1021/acs.jpcc.3c02650>.

15. H. Guan, Y. Lu, J. Liu, et al. Microscopic scaling relation of Ti-based catalysts in de/hydrogenation reactions of Mg/MgH₂. *ACS Catal.* 14(22) (2024) 17159-17170.
<https://doi.org/10.1021/acscatal.4c06122>.
16. H. Liu, X. Duan, Z. Wu, et al. Exfoliation of compact layered Ti₂VAIC₂ MAX to open layered Ti₂VC₂ MXene towards enhancing the hydrogen storage properties of MgH₂. *Chem. Eng. J.* 468 (2023) 143688. <https://doi.org/10.1016/j.cej.2023.143688>.
17. H. Li, J. Li, K. Nie, et al. Single-atom Cu supported on Ti₃C₂T_x for catalyzing hydrogen storage in MgH₂. *J. Phys. Chem. Lett.* 16(14) (2025) 3525-3534. <https://doi.org/10.1021/acs.jpcllett.5c00482>.
18. J. Zhang, W. Wang, X. Chen, et al. Single-atom Ni supported on TiO₂ for catalyzing hydrogen storage in MgH₂. *J. Am. Chem. Soc.* 146(15) (2024) 10432-10442. <https://doi.org/10.1021/jacs.3c13970>.
19. H. Wang, J. Li, X. Wei, et al. Thermodynamic and kinetic regulation for Mg-based hydrogen storage materials: challenges, strategies, and perspectives. *Adv. Funct. Mater.* 34(42) (2024) 2406639. <https://doi.org/10.1002/adfm.202406639>.
20. S. Dong, C. Li, J. Wang, et al. The “burst effect” of hydrogen desorption in MgH₂ dehydrogenation. *J. Mater. Chem. A* 10 (2022) 22363-22372.
21. C. Li, W. Yang, H. Liu, et al. Picturing the gap between the performance and US-DOE’s hydrogen storage target: A data-driven model for MgH₂ dehydrogenation. *Angew. Chem. Int. Ed.* 63(28) (2024) e202320151. <https://doi.org/10.1002/anie.202320151>.
22. Z. Gao, X. Yang, Z. Zhuang, et al. Catalytic strategies and mechanisms for enhancing MgH₂ solid-state hydrogen storage. *Chem Catal.* 6 (2026) 101692.
<https://doi.org/10.1016/j.checat.2026.101692>.
23. J. Cai, H. Wang, X. Tang, et al. Data-driven evidence for the burst effect in MgH₂ dehydrogenation via analysis of experimental kinetic curves. *J. Energy Storage* 136 (2025) 118450.
<https://doi.org/10.1016/j.est.2025.118450>.
24. J. Cai, Y. Jiang, T. Yao, et al. A demand-driven dynamic heating strategy for ultrafast and energy-efficient MgH₂ dehydrogenation utilizing the “burst effect”. *J. Energy Storage* 130 (2025) 117495.
<https://doi.org/10.1016/j.est.2025.117495>.
25. J. Cai, Y. Zhuang, K. Ma, et al. Data-driven discovery of dynamic thermodynamics for dehydrogenation in magnesium-based hydrogen storage materials. *J. Energy Storage* 168 (2026) 122655. <https://doi.org/10.1016/j.est.2026.122655>.
26. T. Yao, Y. Yang, J. Cai, et al. From LLM to Agent: A large-language-model-driven machine learning framework for catalyst design of MgH₂ dehydrogenation. *J. Magnes. Alloy* 14 (2026) 101858.
<https://doi.org/10.1016/j.jma.2025.08.021>.
27. W. Yang, Z. Xu, J. Li, et al. XPEAK: an XRD-driven machine learning platform for predicting the catalyst-enhanced dehydrogenation peak temperature of MgH₂. *J. Mater. Chem. A* 14 (2026) 7579-7595. <https://doi.org/10.1039/D5TA08221H>.

28. Y. Hong, X. Mao. DIVE-to-design: how a multi-agent workflow converts figure-centric literature into an ai-native hydrogen storage discovery engine. *AI Agent* 2 (2026) 2.
<https://dx.doi.org/10.20517/aiagent.2026.04>.
29. A. R. Mishra, J. Pascasio, J. Yang, et al. The rise of the digital materials ecosystem. *AI Agent* 2 (2026) 6. <https://dx.doi.org/10.20517/aiagent.2026.08>.
30. W. Fu, Y. Li, Z. Dong, et al. *Digital Hydrogen-S*: An open-access interactive Data platform for solid-state hydrogen storage materials. *Int. J. Hydrog. Energy* 207 (2026) 153434.
<https://doi.org/10.1016/j.ijhydene.2026.153434>.
31. J. Ma, J. Liu, X. Jiang, et al. A two-dimensional distributed activation energy model for pyrolysis of solid fuels. *Energy*, 230 (2021) 120860. <https://doi.org/10.1016/j.energy.2021.120860>.
32. H. Chen, H. Yu, Q. Zhang, et al. Enhancement in dehydriding performance of magnesium hydride by iron incorporation: A combined experimental and theoretical investigation. *J. Power Sources* 322 (2016) 179-186. <https://doi.org/10.1016/j.jpowsour.2016.05.031>.
33. W. Fu, M. Shu, Y. Liu, et al. Unveiling the micro-mechanism of superior dehydrogenation in γ -MgH₂: Insights into electronic structure of H-Mg bond. *J. Alloy. Compd.* 1036 (2025) 182130.
<https://doi.org/10.1016/j.jallcom.2025.182130>.
34. D. Tan, C. Peng, Q. Zhang. Microstructural characteristics and hydrogen storage properties of the Mg-Ni-TiS₂ nanocomposite prepared by a solution-based method. *Int. J. Hydrog. Energy* 48(44) (2023) 16756-16768. <https://doi.org/10.1016/j.ijhydene.2023.01.185>.
35. S. Wu, Y. Chen, W. Kang, et al. Hydrogen storage properties of MgTiVZrNb high-entropy alloy and its catalytic effect upon hydrogen storage in Mg. *Int. J. Hydrog. Energy* 50 (2024) 1113-1128.
<https://doi.org/10.1016/j.ijhydene.2023.09.022>.
36. J. Wu, Z. Liu, H. Zhang, et al. Hydrogen storage performance of MgH₂ under catalysis by highly dispersed nickel-nanoparticle-doped hollow spherical vanadium nitride. *J. Magnes. Alloy* 12(12) (2024) 5132-5143. <https://doi.org/10.1016/j.jma.2023.11.010>.
37. Z. Lan, H. Liang, X. Wen, et al. Experimental and theoretical studies on two-dimensional vanadium carbide hybrid nanomaterials derived from V₄AlC₃ as excellent catalyst for MgH₂. *J. Magnes. Alloy* 11(10) (2023) 3790-3799. <https://doi.org/10.1016/j.jma.2022.09.019>.
38. Z. Liu, H. Ning, R. Liu, et al. Fabrication of V₂O₃-TiO₂-rGO ternary heterojunction composite to enhance the hydrogen storage performance of MgH₂. *Chem. Eng. J.* 499 (2024) 155877.
<https://doi.org/10.1016/j.cej.2024.155877>.
39. J. Zhang, C. Zheng, Y. Wang, et al. Effect of La-Ni@₃DG catalyst concentration on the hydrogen storage properties of MgH₂. *Int. J. Hydrog. Energy* 95 (2024) 666-677.
<https://doi.org/10.1016/j.ijhydene.2024.11.016>.
40. H. Wan, X. Yang, S. Zhou, et al. Enhancing hydrogen storage properties of MgH₂ using FeCoNiCrMn high entropy alloy catalysts. *J. Mater. Sci. Technol.* 149 (2023) 88-98.
<https://doi.org/10.1016/j.jmst.2022.11.033>.

41. X. Lu, L. Zhang, H. Yu, et al. Achieving superior hydrogen storage properties of MgH_2 by the effect of TiFe and carbon nanotubes. *Chem. Eng. J.* 422 (2021) 130101. <https://doi.org/10.1016/j.cej.2021.130101>.
42. D. Khan, J. Zou, S. Panda, et al. Mechanism of Thermodynamic Destabilization and Fast Desorption Kinetics in a Mechanically Alloyed MgH_2 -In Composite. *J. Phys. Chem. C* 124(18) (2020) 9685-9695. <https://doi.org/10.1021/acs.jpcc.0c00305>.
43. B. Zhang, X. Xie, Y. Wang, et al. In situ formation of multiple catalysts for enhancing the hydrogen storage of MgH_2 by adding porous $\text{Ni}_3\text{ZnC}_{0.7}/\text{Ni}$ loaded carbon nanotubes microspheres. *J. Magnes. Alloy* 12(3) (2024) 1227-1238. <https://doi.org/10.1016/j.jma.2022.07.004>.
44. C. Lu, H. Liu, L. Xu, et al. Two-dimensional vanadium carbide for simultaneously tailoring the hydrogen sorption thermodynamics and kinetics of magnesium hydride. *J. Magnes. Alloy* 10(4) (2022) 1051-1065. <https://doi.org/10.1016/j.jma.2021.03.030>.
45. Y. Jiang, N. Si, W. Jiang, et al. FeNiCu-based composite catalyst for hydrogen storage in MgH_2 . *Chem. Eng. J.* 499 (2024) 156449. <https://doi.org/10.1016/j.cej.2024.156449>.
46. M. Song, F. Wu, Y. Jiang, et al. Optimizing FeCoNiCrTi high-entropy alloy with hydrogen pumping effect to boost de/hydrogenation performance of magnesium hydride. *Rare Met.* 43(7) (2024) 3273-3285. <https://doi.org/10.1007/s12598-024-02703-y>.
47. Wang P, Wang Z, Tian Z, et al. Enhanced hydrogen absorption and desorption properties of MgH_2 with NiS_2 : The catalytic effect of in-situ formed MgS and Mg_2NiH_4 phases, *Renew. Energy*. 160 (2020) 409-417. <https://doi.org/10.1016/j.renene.2020.07.014>.
48. Yan C, Lu X, Zheng J, et al. Dual-cation K_2TaF_7 catalyst improves high-capacity hydrogen storage behavior of MgH_2 . *Int. J. Hydrog. Energy* 48(15) (2023) 6023-6033. <https://doi.org/10.1016/j.ijhydene.2022.11.191>.
49. Chen Y, Shao Y, Liu Y, et al. Catalysis derived from three-dimensionally ordered microporous Nb_2O_5 towards the hydrogen storage performance of magnesium hydride. *Fuel* 364 (2024) 131025. <https://doi.org/10.1016/j.fuel.2024.131025>.
50. Yang T, Li Q, Liu N, et al. Improved hydrogen absorption and desorption kinetics of magnesium-based alloy via addition of yttrium. *J. Power Sources* 378 (2018) 636-645. <https://doi.org/10.1016/j.jpowsour.2018.01.003>.
51. Yong H, Guo S, Yuan Z, et al. Catalytic effect of in situ formed Mg_2Ni and REH_x (RE: Ce and Y) on thermodynamics and kinetics of Mg-RE-Ni hydrogen storage alloy. *Renew. Energy* 157 (2020) 828-839. <https://doi.org/10.1016/j.renene.2020.05.043>.
52. T. Si, Y. Cao, Q. Zhang, et al. Enhanced hydrogen storage properties of a Mg-Ag alloy with solid dissolution of indium: a comparative study. *J. Mater. Chem. A* 3 (2015) 8581-8589. <https://doi.org/10.1039/C5TA00292C>.
53. T. He, X. Wang, H. Liu, et al. Enhanced hydrogen desorption/absorption properties of magnesium hydride with $\text{CeF}_3@ \text{Gn}$. *Int. J. Hydrog. Energy* 45(7) (2020) 4754-4764.

<https://doi.org/10.1016/j.ijhydene.2019.12.111>.

54. Y. Li, L. Ren, Z. Li, et al. Achieving wide-temperature-range physical and chemical hydrogen sorption in a structural optimized Mg/N-doped porous carbon nanocomposite. *Nano-Micro Lett.* 18 (2025) 94. <https://doi.org/10.1007/s40820-025-01931-w>.
55. M. Chen, X. Xiao, X. Wang, et al. Self-templated carbon enhancing catalytic effect of ZrO_2 nanoparticles on the excellent dehydrogenation kinetics of MgH_2 . *Carbon* 166 (2020) 46-55. <https://doi.org/10.1016/j.carbon.2020.05.025>.
56. C. Liu, Z. Yuan, W. Li, et al. Improved hydrogen storage performance of MgH_2 by adding CeO_2 @NC with high catalytic activity. *J. Mater. Sci. Technol.* 238 (2025) 119-131. <https://doi.org/10.1016/j.jmst.2025.02.066>.
57. C. Peng, Y. Li, Q. Zhang. Amorphous mixed transition metal oxides: A novel catalyst for boosting dehydrogenation of MgH_2 . *Scr. Mater.* 248 (2024) 116149. <https://doi.org/10.1016/j.scriptamat.2024.116149>.
58. L. Ren, Y. Li, Z. Li, et al. Boosting hydrogen storage performance of MgH_2 by oxygen vacancy-rich $\text{H-V}_2\text{O}_5$ nanosheet as an excited H-pump. *Nano-Micro Lett.* 16 (2024) 160. <https://doi.org/10.1007/s40820-024-01375-8>.
59. A. Bhatnagar, S. Pandey, A. Vishwakarma, et al. Fe_3O_4 @graphene as a superior catalyst for hydrogen de/absorption from/in MgH_2 /Mg. *J. Mater. Chem. A* 4 (2016) 14761-14772. <https://doi.org/10.1039/C6TA05998H>.
60. L. Wang, L. Zhang, X. Lu, et al. Surprising cocktail effect in high entropy alloys on catalyzing magnesium hydride for solid-state hydrogen storage. *Chem. Eng. J.* 465 (2023) 142766. <https://doi.org/10.1016/j.cej.2023.142766>.
61. S. Guemou, F. Wu, P. Chen, et al. Graphene-anchored Ni_6MnO_8 nanoparticles with steady catalytic action to accelerate the hydrogen storage kinetics of MgH_2 . *Int. J. Hydrog. Energy* 48(62) (2023) 23943-23955. <https://doi.org/10.1016/j.ijhydene.2023.03.243>.
62. N. Xu, K. Wang, Y. Zhu, et al. PdNi biatomic clusters from metallene unlock record-low onset dehydrogenation temperature for bulk- MgH_2 . *Adv. Sci.* 35 (2023) 2303173. <https://doi.org/10.1002/adma.202303173>.
63. H. Guan, J. Liu, X. Sun, et al. Titanium-nickel dual active sites enabled reversible hydrogen storage of magnesium at 180 °C with exceptional cycle stability. *Adv. Mater.* 37(26) (2025) 2570178. <https://doi.org/10.1002/adma.202570178>.
64. Z. Tian, Z. Wang, P. Yao, et al. Hydrogen storage behaviors of magnesium hydride catalyzed by transition metal carbides. *Int. J. Hydrog. Energy* 46(80) (2021) 40203-40216. <https://doi.org/10.1016/j.ijhydene.2021.09.212>.
65. P. Wang, Z. Tian, Z. Wang, et al. Improved hydrogen storage properties of MgH_2 using transition metal sulfides as catalyst. *Int. J. Hydrog. Energy* 46(53) (2021) 27107-27118. <https://doi.org/10.1016/j.ijhydene.2021.05.172>.

Figures

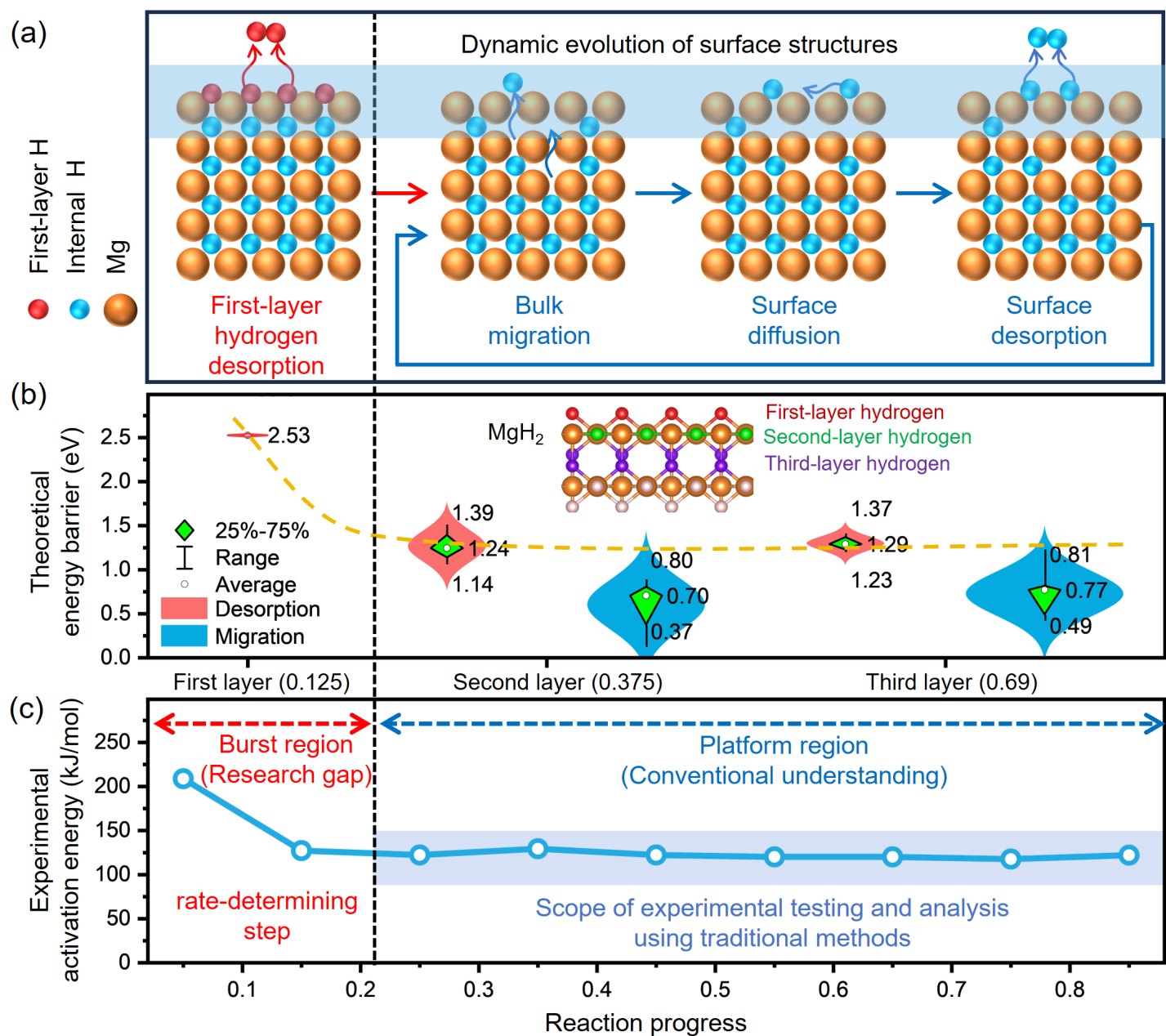


Figure 1

Microscopic origin and macroscopic identification of the burst effect in MgH₂ dehydrogenation. (a) Dynamic evolution of the MgH₂ surface during dehydrogenation, (b) layer-dependent barriers for hydrogen desorption and migration and (c) dehydrogenation activation energy curve and characteristic parameters.

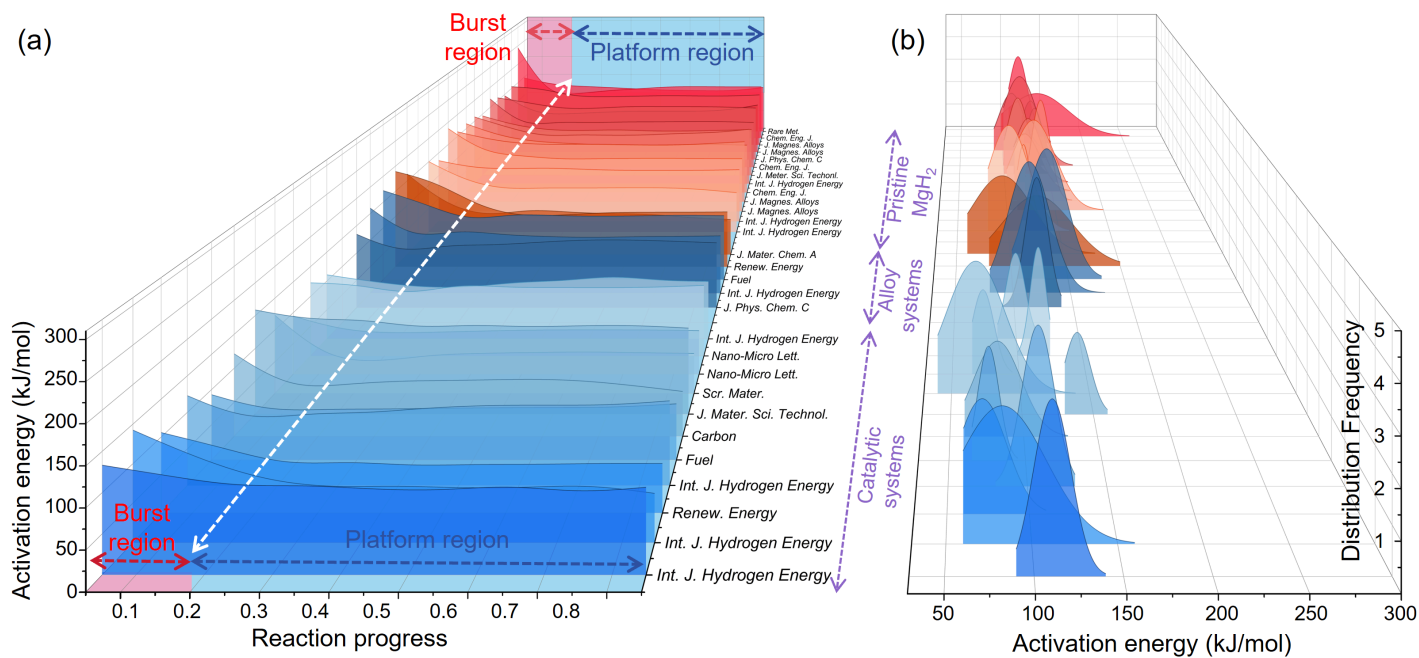


Figure 2

Database-enabled statistical validation of the burst effect across Mg-based systems [34-58]. (a) Reconstructed dehydrogenation activation energy curves for representative Mg-based systems and (b) statistical distribution of dynamic activation energies across Mg-based systems.

