UDC 621.45

INTEGRATING FIRST-PRINCIPLES DISCOVERY AND SOLAR-THERMAL REACTOR DESIGN FOR SUSTAINABLE HYDROGEN-RICH SYNGAS PRODUCTION FROM BIOMASS

Yixing Du[1], Yongqi Jiao[1,2], Dan Zhu[1,2], Lei Han[1], Lifeng Li[1], Yong Shuai[1,2], Bo Wang[1*]
[1] School of Energy Science and Engineering, Harbin Institute of Technology, Harbin, 150001, China
[2] Zhengzhou Research Institute, Harbin Institute of Technology, Zhengzhou, 450003, China
* Corresponding author: bo.wang@hit.edu.cn

Keywords: solar-driven biomass gasification, thermochemical hydrogen production, perovskite oxides, B-site doping, hybrid radiative heating

The transition to sustainable propulsion and power generation demands high-efficiency, low-carbon pathways for converting renewable resources into clean fuels [1]. This work integrates two complementary advances: a first-principles investigation of B-site-doped $LaCoO_3$ perovskites for thermochemical water splitting and a solar-driven biomass gasifier with hybrid direct-indirect radiative heating [2]. The integrated analysis provides theoretical guidelines for designing next-generation biomass-to-syngas conversion systems with enhanced energy efficiency and product quality.

The DFT+U study systematically examines the effect of B-site dopants (Ga, Cr, Ti, Zr, Nb) on oxygen-vacancy-assisted H_2O splitting on $LaCo_{0.75}M_{0.25}O_3$ (001) surfaces (see Fig.). While H_2O dissociation is thermodynamically favorable on all defective surfaces, hydrogen migration constitutes the main kinetic barrier. The calculated H migration barriers decrease from 3.40 eV (Ga) and 2.90 eV (Cr) to 2.65 eV (Ti) and ~2.50 eV (Zr, Nb), demonstrating that Ti and Nb substantially lower the energy cost for hydrogen mobility. Electronic structure analysis reveals that stronger Co 3d–O 2p coupling in Ga and Cr stabilizes the dissociated hydroxylated configuration but increases the H migration penalty. Oxygen migration barriers below 0.3 eV indicate facile near-surface oxygen redistribution. Ab initio molecular dynamics at 1100 K confirms rapid H_2O dissociation within 5 ps, while H_2 formation is not observed, corroborating that H migration is the limiting step. Ti and Zr emerge as balanced alternatives to the Ga-doped baseline, whereas Nb is less favorable under high-temperature reconstruction.

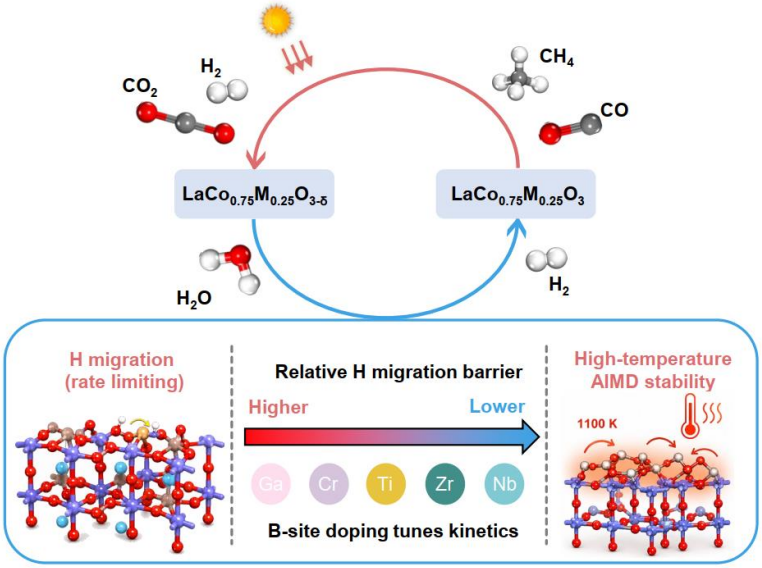

Fig. 1 – Overview of thermochemical water splitting and the computational strategy for evaluating B-site-doped $LaCoO_3$ surfaces.

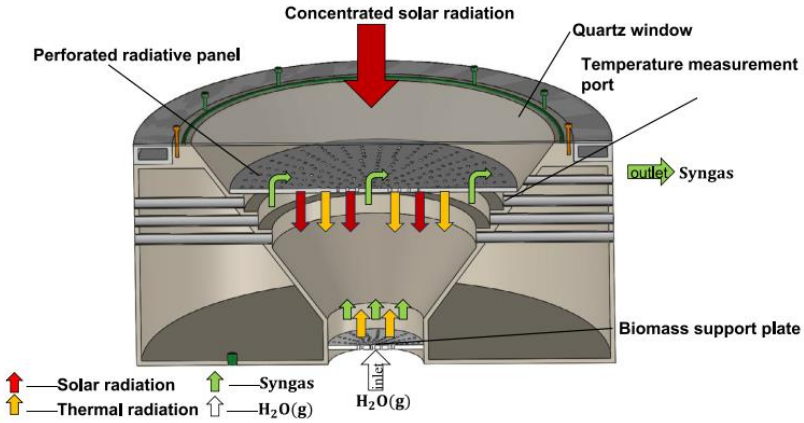

Fig. 2 – Schematic of a solar-driven biomass gasifier for H_2 production

In parallel, a novel solar-driven biomass gasifier is proposed and theoretically evaluated (see

Fig.). The gasifier integrates a perforated SiC radiative panel to create an adjustable hybrid heating mode, combining the high solar absorption efficiency of direct irradiation with the operational stability of indirect heating. An energy-partitioning Monte Carlo radiative model is coupled with a Gibbs free energy minimization chemical equilibrium model for poplar sawdust gasification. The relative error in required solar input between Gaussian and uniform irradiation profiles increases nonlinearly from 0.6% (φ = 0.1) to 4.7% (φ = 0.9), validating the necessity of high-fidelity Gaussian modeling. Increasing the biomass reaction temperature (T_{bio}) from 800 K to 1300 K monotonically decreases the H_2/CO molar ratio from 4.7 to 1.6, while the carbon conversion rate approaches unity and the energy upgrade factor U rises from 0.94 to 1.25. An optimal T_{bio} window of 950–1100 K is identified, ensuring near-complete carbon conversion and high syngas quality. Multi-objective optimization reveals a synergistic optimum where high energy conversion efficiency coincides with the ideal H_2/CO ratio of 2.0 required for Fischer–Tropsch synthesis and methanol production, achieved at $T_{bio} \approx 995$ K and high perforation ratios. The peak energy upgrade factor approaches 1.25, demonstrating effective solar energy storage in chemical bonds

Crucially, the DFT-derived material design principles align with the reactor-level operational needs. The low hydrogen migration barriers predicted for Ti- and Zr-doped perovskites directly support the efficient hydrogen evolution required to achieve the H2/CO = 2.0 target in the solar gasifier. Furthermore, the facile oxygen migration (<0.3 eV) indicates that these doped oxides can serve as effective oxygen carriers or catalytic surfaces for in-situ tar cracking and water–gas shift enhancement within the high-temperature (≥1573 K) perforated panel zone. This integration provides a pathway from atomic-scale dopant selection to macroscopic reactor optimization.

This combined theoretical framework establishes foundational knowledge for developing advanced biomass power plants and sustainable hydrogen production systems. Future work will focus on experimental validation of the optimal Ti/Zr-doped LaCoO3 in the hybrid solar gasifier prototype, followed by techno-economic and life-cycle assessments for industrial-scale propulsion and power applications.

References

1. Xu, D., Wang, B., Li, X., Cheng, Y.W., Fu, W., Dai, Y., Wang, C.-H., Solar-driven biomass chemical looping gasification using Fe3O4 for syngas and high-purity hydrogen production, Chemical Engineering Journal 479(7411), 2024, 147901.

2. Jiao, Y., Zhu, D., Liu, D., Li, L., Dong, S., Jiang, X., Ok, Y.S., Rafique, M., Wang, B., A solar-driven biomass gasifier with bimodal radiative heating: Heat transfer characteristics and operational parameter optimisation, Energy 340, 2025, p. 139060.