Title: Hydrogen Production via Methane Reforming: Experimental and Theoretical Analysis Using Flower-Shaped CeO_2 Catalysts with Ni Nanoparticles

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Low-cost hydrogen production is crucial for driving the widespread use of fuel cells, renowned for their high power generation efficiency[1]. My research addresses this challenge by focusing on methane produced from organic waste fermentation, specifically shrimp farming residues, as an affordable hydrogen carrier. In collaboration with Vietnam, a joint test site has been established to showcase methane production and hydrogen extraction, as depicted in Figure 1[2].

My contribution centers on the theoretical design of catalysts for efficient hydrogen extraction from methane. Using density functional theory (DFT) and experimental validation, I calculated the activation barriers for methane dissociation on CeO_2-supported Ni nanoparticles. Through the Vienna ab initio simulation package (VASP) and the nudged elastic band (NEB) method, I analyzed various Ni nanoparticle configurations on CeO_2 (111) surfaces to uncover the mechanisms driving methane dissociation in the dry reforming of methane (DRM) reaction.

The results reveal activation barriers for methane dissociation ranging from 0.80 eV to 1.03 eV, closely aligning with experimental values (0.67 eV). Furthermore, the study indicates that increasing the positive charge of Ni nanoparticles could significantly enhance methane dissociation, offering a promising pathway for optimizing catalysts in DRM processes and advancing efficient hydrogen production[3].

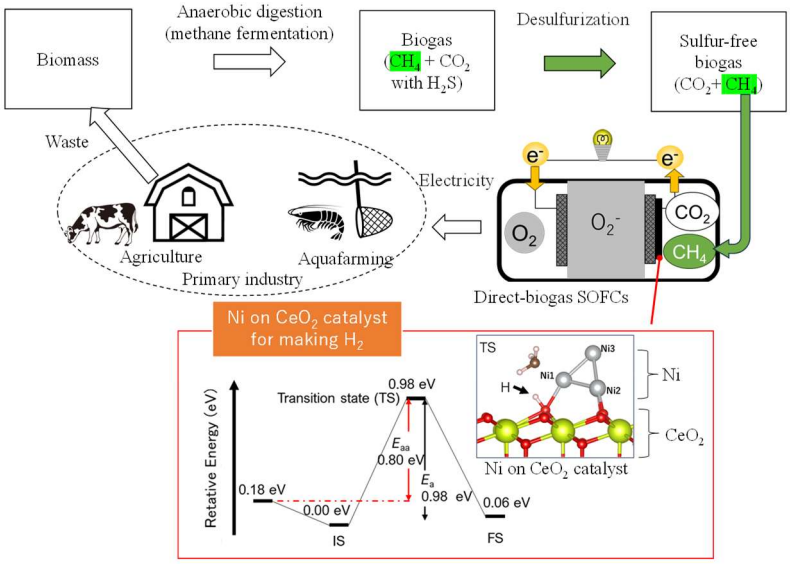

Figure 1. Energy circulation model combining primary industry and fuel cells and the role of Ni nanoparticle catalysts

References:

[1] Y. Shiratori et al., Fuel Cells 19, 346-353 (2019).
[2] P. H. Tu et al., Fuel Cells, 1-11 (2024).
[3] T. Fujisaki et al., Phys. Chem. Chem. Phys, (2025)

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