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HPC Applications Enabling Catalysis Design for Ammonia Decomposition to Produce Hydrogen

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The envisaged hydrogen economy cannot be realized without a proactive approach to novel materials design. Hydrogen is emerging as a game changer in the grand realm of clean energy value chain mainly because, as an energy vector, hydrogen is both an energy carrier and an energy source. However, despite this potential, several challenges limit large scale adoption of hydrogen including the fact that hydrogen is explosive and flammable, making it difficult to store and transport. One way of mitigating this bottleneck is chemical storage in molecular carriers. On this, liquid organic hydrogen carriers have gained dominance. However, they have not reached the level of technological maturity for large scale development and adoption. Molecules such as ammonia are likely to be good alternatives since their value chain is technologically mature and they can be used as feedstock in hydrogen production. Hydrogen is produced from ammonia mainly through catalytic decomposition. The rational design of novel catalysts for ammonia dehydrogenation is not feasible via —trial and error— experimental investigations and is also computationally intensive. Hence the need for high-performance computing (HPC). With HPC coupled with density functional theory models, it is feasible for one to high-throughput screen of different catalytic processes involved in hydrogen production via catalytic decomposition, compared to conventional laboratory-based catalyst synthesis and optimization which are known to be costly, time-consuming, and wasteful in terms of materials.

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