



Designing Promoted Pt/ θ - δ -Al₂O₃ Catalysts for Perhydro Benzyltoluene Dehydrogenation Using Bayesian Optimization

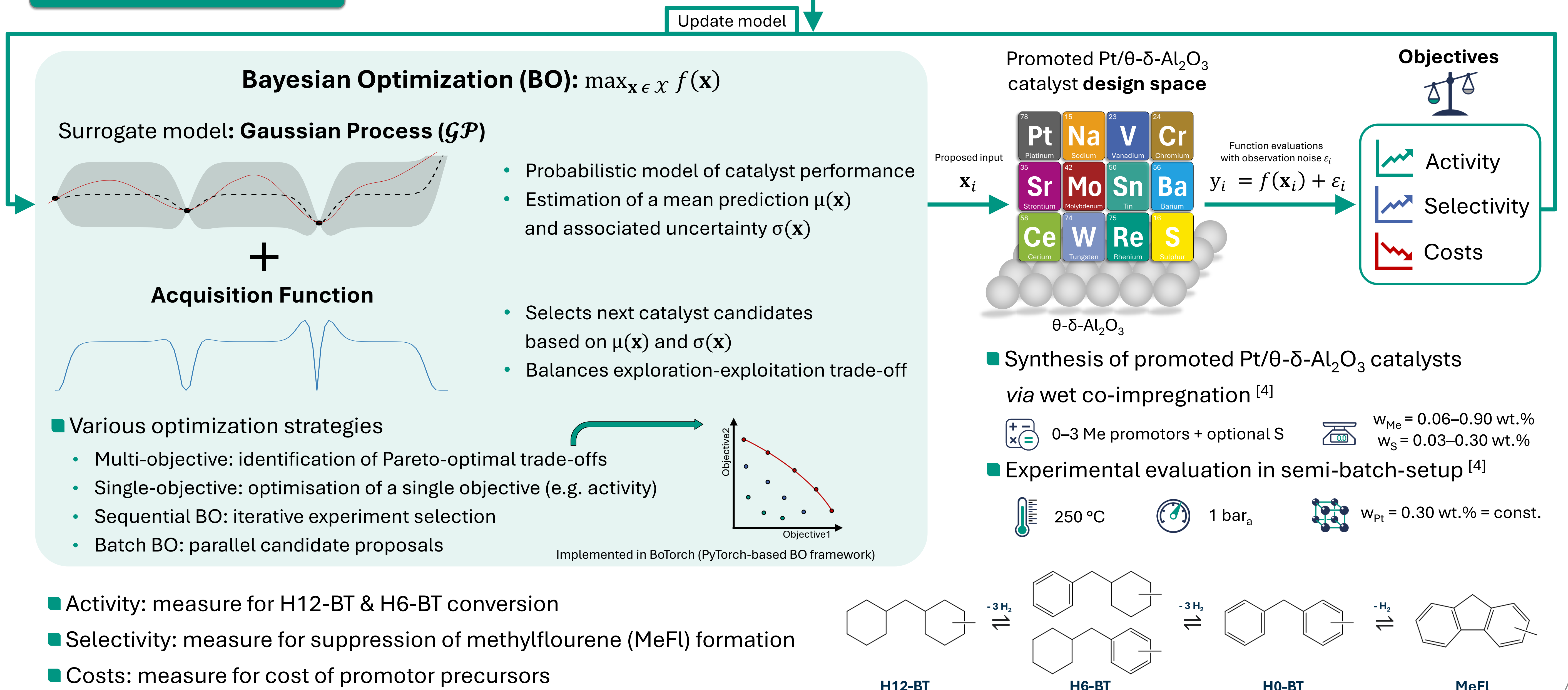
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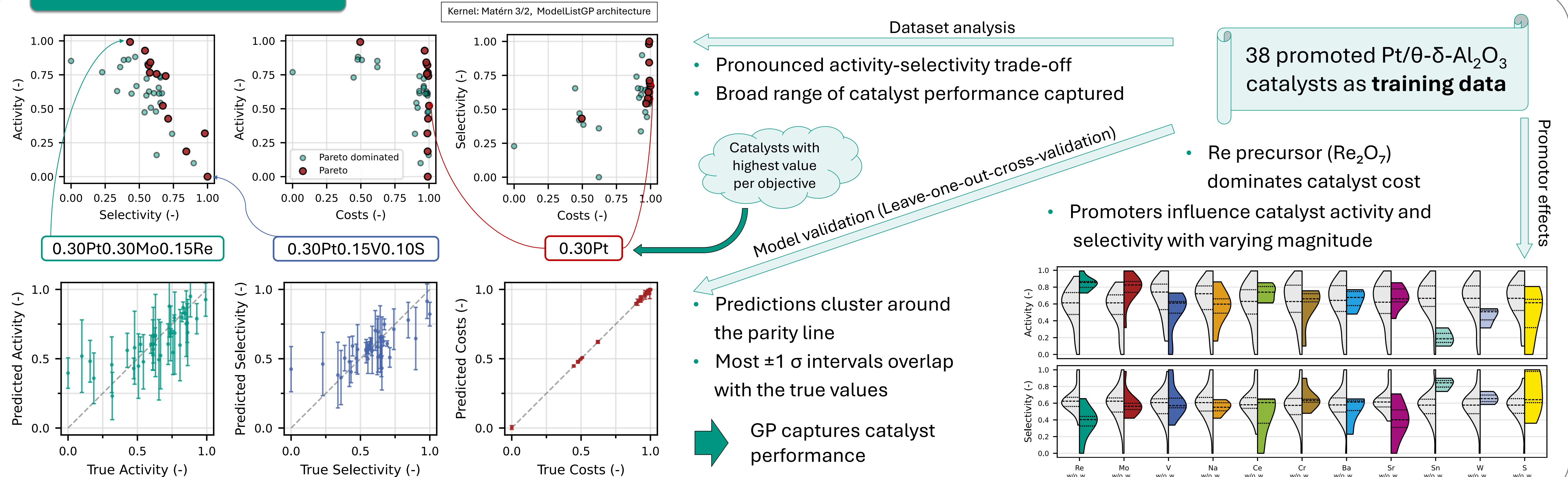
MOTIVATION

- Chemical hydrogen storage in Liquid Organic Hydrogen Carriers (LOHCs)
 - Increase of volumetric energy density; safe and stable liquid for handling^[1]
 - Perhydro benzyltoluene/benzyltoluene (H12-BT/H0-BT) as potential LOHC system
- Promotion of Pt/ θ - δ -Al₂O₃ catalysts to increase catalyst performance
 - Extensive literature on promoter effects in H12-BT dehydrogenation^[2-4]
 - Multi-promoter systems enable tuning of activity and selectivity
 - High-dimensional black-box optimisation problem with constraints
- Bayesian Optimization of catalyst design
 - Data and sample-efficient optimization for expensive experimental systems
 - Identification of promising catalyst candidates with few experiments
 - Efficient exploration of large catalyst design space

APPROACH



RESULTS



OUTLOOK

- Systematic Bayesian Optimization of catalyst composition
- Extension of design space: Pt loading, promotor set, support material

REFERENCES & ACKNOWLEDGEMENTS

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 [2] K. Alconada, V. L. Barrio, *Appl. Catal. B*, **2024**, 357, 124349
 [3] K. Alconada, V. L. Barrio, *Int. J. Hydrog. Energy*, **2024**, 51, 243-255
 [4] D. Strauch, P. Weiner, B. B. Sarma, et al., *M. Wolf, Catal. Sci. Technol.* **2024**, 14, 1775.

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