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Catalysis: Reactivity and Structure

As shown in Fig. 1, the predicted YSIs show good agreement with measurements, except for 2,5-dimethylfuran. We also quantify the sensitivity of the YSI predictions to aromatic growth reactions and ...

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In addition, a quantitative YSI formulation is also derived in ReaxFF and the ReaxFF-predicted YSI values are compared with measurement data and reasonably good ... for fuels with unknown or ...

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systems analysis, experimental design, and mathematical modeling; (5) automatic data. storage, retrieval, manipulation, and (form of) output; and (6) communication. Additional Conclusions and ...

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