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Communication

Rational design of FLP catalysts for reversible H₂ activation: A DFT study of the geometric and electronic effects

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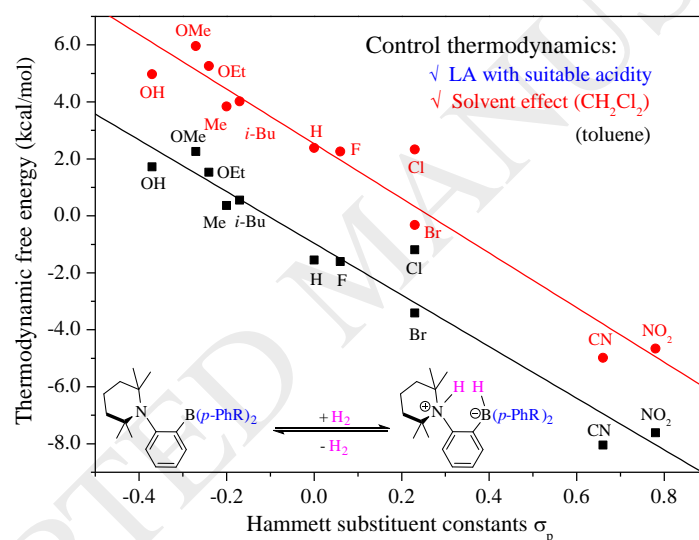
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Graphical abstract



The thermodynamics of reversible H₂ activation could be controlled by adjusting substituents of LA group and using different polar solvents, which forges a guide to design potential FLPs catalysts for reversible H₂ activation.

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