

LOW-TEMPERATURE LIQUID METAL CATALYSTS

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A new type of catalyst has recently emerged in both experimental and computational literature: low-temperature liquid metals.¹ These promising materials, including Ga and its alloys, are defined by their ability to melt close above room temperature, while still maintaining metallic character and behaviour.² Several high-profile reports from the recent years have demonstrated that liquid metal catalysts can offer unprecedented advantages in activity,³ stability,⁴ and selectivity⁵ over their traditional solid counterparts.

Despite the notable degree of attention directed towards liquid metal catalysts, the vast majority of work in this area has been experimental in nature,^{4,5} and atomic-scale insight is often limited. This can be partly attributed to the difficulty in studying a dynamic and changing liquid with methods such as density functional theory. As a result, modelling studies have been limited to describing catalysis on static snapshots, or reconstructed solid surfaces, which are unable to fully capture the dynamic nature of a liquid catalyst. In this work, we report recent methodological developments using *ab initio* molecular dynamics as a sampling technique to probe reactions on liquid metal catalysts. We show that the adsorption energies of intermediates will vary over time, based on the transient geometry of the liquid metal surface, and we demonstrate how this can allow intermediates to interconvert with lower energy gaps than previously predicted.

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