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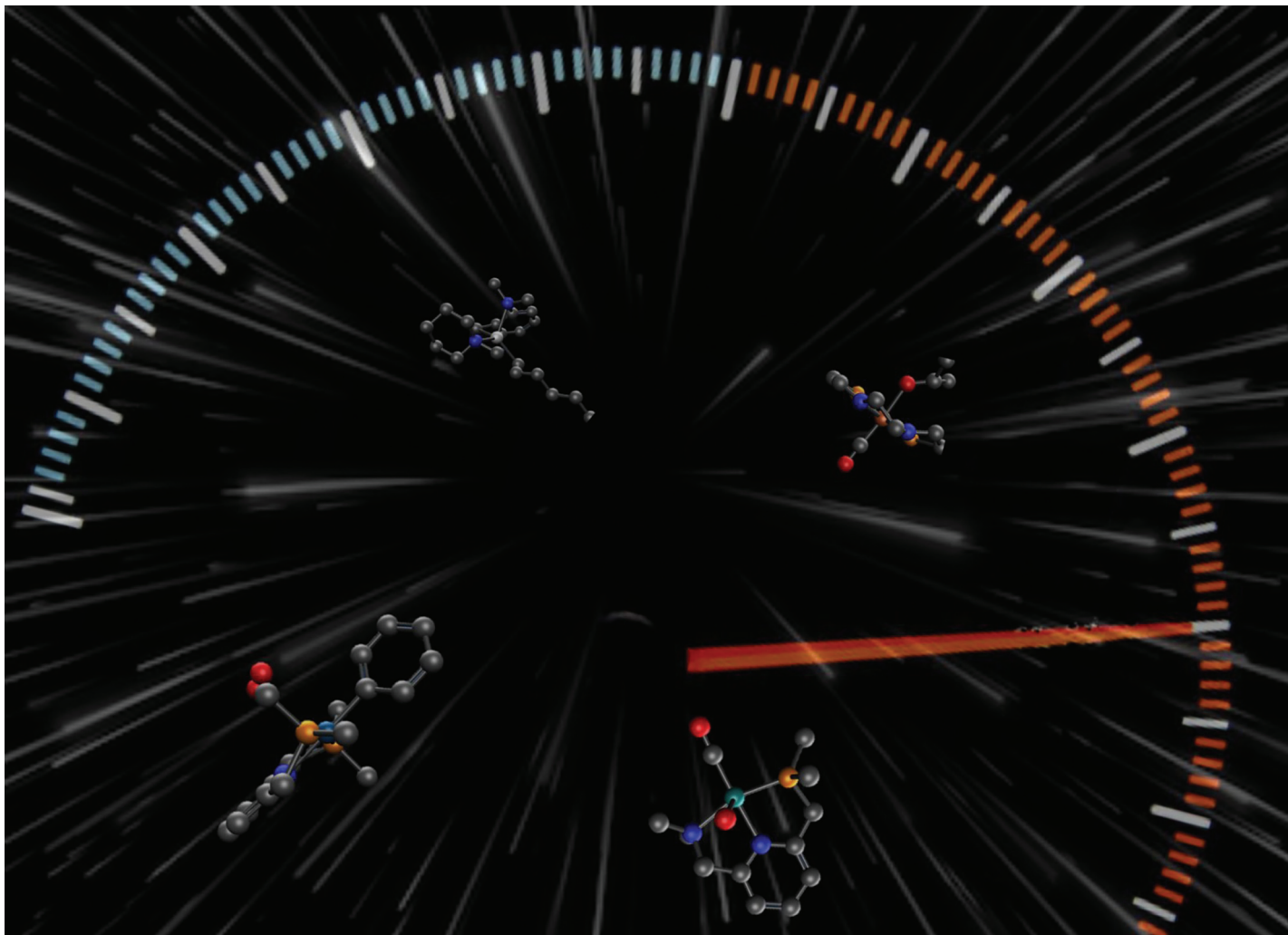
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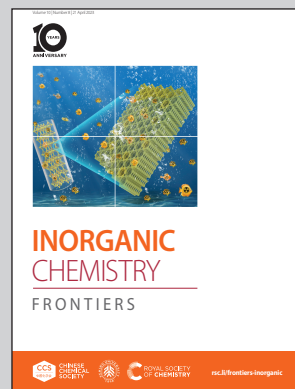


Showcasing research from Dr Marcelo T. de Oliveira and co-workers, Department of Chemistry and Physics, La Trobe Institute of Molecular Sciences.

Accelerating computations of organometallic reaction energies through hybrid basis sets

A straightforward hybrid basis set approach to compute organometallic reaction energies is described to reduce computational times by up to 10-fold while maintaining the accuracy of DFT results.

As featured in:



See Marcelo T. de Oliveira *et al.*, *Inorg. Chem. Front.*, 2023, **10**, 2262.

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