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Minimum energy pathways from Quantum Monte Carlo

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We perform quantum Monte Carlo calculations to determine minimum energy pathways of simple chemical reactions, and compare the computed geometries and reaction barriers with those obtained with density functional theory and quantum chemistry methods. We find that QMC performs in general significantly better than DFT, being also able to treat cases in which DFT is inaccurate or even unable to locate the transition state. Since the wave function form employed here is particularly simple and can be transferred to larger systems, we suggest that a QMC approach is both viable and useful for reactions difficult to address by DFT and system sizes too large for high level quantum chemistry methods.