



The Abdus Salam  
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for Theoretical Physics**



## **16th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods**

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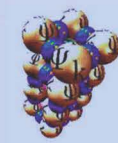
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*Workshop Website:*

[http://cdsagenda5.ictp.it/full\\_display.php?ida=a12161](http://cdsagenda5.ictp.it/full_display.php?ida=a12161)

# Minimum energy pathways from Quantum Monte Carlo

*S. Saccani*<sup>1</sup>, *C. Filippi*<sup>2</sup>, *S. Moroni*<sup>1</sup>,

1. SISSA and DEMOCRITOS National Simulation Center, IOM-CNR, Trieste, Italy
2. MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

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.