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Recent advances in quantum Monte Carlo: Applications to lithium ion – Stockmayer clusters, hydrogen isotopic separation, and the investigation of excited state manifolds

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Over the past two decades, our group at Arcadia University and the Mella group at Università degli Studi dell'Insubria, have been closely collaborating in the development and implementation of quantum Monte Carlo methods, primarily to estimate nuclear quantum effects in condensed matter and clusters. The most recent advances include the formal development of path integral and diffusion Monte Carlo methods that permit enhanced convergence when rigid constraints are included in simulations, the introduction of Smart-Darting-like techniques to enhance the sampling of the ground state density in extremely frustrated systems, and the exploration of the mathematical property of the Langevin equation in manifolds with boundaries and gradient torsion associated with nodal surfaces of excited states. Application examples include the determination of coupling effects on the ground state of gas phase molecules between rotation and torsional degrees of freedom, the determination of the ground state energy and wave functions of lithium-ion Stockmayer clusters, the enhancement of hydrogen isotopic separation offered by the surface of ammonia clusters, the ring polymer molecular dynamics from the Brownian bridge representation of the path integral, and the simulation of multi-electronic states in the Kustaanheimo-Stiefel Space by Diffusion Monte Carlo.



Fig. 1 The capped pentagonal bipyramid global minimum of the 5-D PES of $(\text{H}_2)_{10}$

Biography

Emanuele Curotto completed his Bachelor of Science at University of Massachusetts Lowell; Doctorate degree at Yale University in 1996 under the direction of Dr. J Cross, and; was a Postdoctoral fellow at University of Rhode Island under the direction of Dr. D L Freeman. He currently serves as Professor and Department Chair at Arcadia University (formerly Beaver College).

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