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Large-scale Quantum Calculations of Inelastic and Reactive Scattering in Cold and Ultracold Gases[1]

BALAKRISHNAN NADUVALATH, University of Nevada Las Vegas

Recent advances in cooling and trapping atomic and molecular systems have led to exciting opportunities for the investigation of inelastic and reactive collisions in ultra cold gases. This opens up novel possibilities for the control and manipulation of chemical reaction dynamics and molecular scattering events in the extreme quantum regime. Quantum coupled-channel calculations have become the preferred approach to describe these events theoretically. While such calculations can be performed routinely for triatomic systems composed of light atoms, they become computationally intractable as the size and dimensionality of the system increase. Even for triatomic systems, calculations become prohibitive when all internal quantum numbers, including, rotation, vibration, spin and hyperfine levels are considered. I will discuss recent progress in inelastic and reactive collisions of atom-diatom and diatom-diatom systems at cold and ultra cold temperatures and delineate challenges involved in moving beyond three and four atomic systems. I will further discuss how these problems could be tackled with emerging advances in CPU/GPU architectures and availability of petascale computational platforms.

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